Appendix A

Data Inputs for Phase II Groundwater Modeling

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Appendix A
Data Inputs for Phase II Groundwater Modeling

This appendix documents the inputs used in the groundwater modeling. In addition, Attachment A.1 provides additional methodological details for IWEM. Note that Attachment A.1 is a memo with its own attachments A and B; for clarity, those attachments are labeled as "Memo Attachment A" and "Memo Attachment B."

A.1 Scenarios

Table A-1 summarizes the source scenarios modeled. For nonaerated units, EPA did one central-tendency run, in which all WATER9 inputs were set to central-tendency values, and four high-end runs, in which two of the most critical inputs were set to high-end values. All other inputs, including all waste parameters, were set to central-tendency values for all runs. The most sensitive parameters for nonaerated units are biomass, flow, capacity, and solids removal efficiency (fraction of diverted flow that is solids).

For the aerated treatment train, biomass was not varied because a very low value would not be realistic, because such treatment trains are designed to support the growth of biomass. Solids parameters are not an input to the aerated treatment train units in WATER9. Thus, there were only two critical parameters for the aerated treatment train: flow and residence time. EPA did one central-tendency run and two high-end runs, with one of these two critical parameters set to high end for each run.

Table A-1. Summary of Source Scenarios Modeled

	Scenario							
	Nonaerated Units					Aerated Treatment Train		
Component	1	2	3	4	5	7	8	9
Biomass	high	central	high	central	high	not varied	not varied	not varied
Flow	central	central	high	high	central	central	high	central
Capacity/ residence time	high	central	central	high	central	central	central	high
Solids	central	central	central	central	high	NA	NA	NA

A.2 Source Inputs

A.2.1 Data Sources

EPA used four primary sources of data:

- BRS database—waste flows
- SIS survey database—unit characteristics for surface impoundments and waste characteristics
- Tanks database (U.S. EPA, 1987)—unit characteristics for tanks
- WATER9 default values—parameters not available from the other sources.

The BRS data are the data reported by facilities to EPA on quantities of hazardous wastes managed. EPA pulled BRS data on waste volumes by facility and by waste stream of the F002 and F005 waste streams being considered for exemption. For the risk modeling, EPA used the facility-level data, assuming that most facilities would combine these small waste streams for treatment or storage.

The SIS survey database (U.S. EPA, 2001) is the most comprehensive available data set on Subtitle D (nonhazardous) surface impoundments. Although the universe of impoundments in the database was sampled specifically for SIS in-scope impoundments, the database has undergone extensive quality assurance checks and is being used in other Office of Solid Waste (OSW) work. In using the SIS survey data, EPA limited the universe to impoundments that manage at least one organic chemical (not necessarily one of the three analyzed in this assessment). EPA has taken this approach before (most recently to assess default values for the Industrial Waste Air Model (IWAIR)) to weed out impoundments managing only inorganics, which tend to be rather different than those that manage organics. EPA pulled the data needed and calculated weighted medians for each parameter, using the survey weights. The SIS data include volume, flow, area, depth, and most of the needed waste characteristics.

The Tanks database was developed for the Air Characteristic Study and also used for the Paints listing (RTI, 2001). The database is based on EPA's National Survey of Hazardous Waste Treatment, Storage, Disposal, and Recycling Facilities (TSDR) survey (U.S. EPA, 1987) and, therefore, reflects hazardous waste units rather than Subtitle D facilities. However, EPA believes these are the only data currently available for characterizing tanks. The Tanks database does not have associated weights, so those data were used unweighted. The database contains data on the volume of the tank and the quantity of hazardous and nonhazardous waste managed. The Tanks database does not contain data on area or depth. It also does not include waste characteristic data; therefore, we used the SIS data to characterize the waste, on the assumption that the waste streams are similar regardless of whether they are managed in a tank or a surface impoundment.

The WATER9 default values are based on engineering principles and were used in this analysis only for parameters to which the model is not highly sensitive, when data were not readily available from other sources.

A.2.2 Unit Characterization

A.2.2.1 Nonaerated units. Many of the parameters used in WATER9 are interrelated and cannot be set independently without producing an inconsistent data set. For example, a very large waste volume would not be likely to be managed in a very small unit. Similarly, volume of the unit and dimensions, such as area and depth, are related but not to the degree of having a fixed mathematical relationship. The goal was to choose, for each scenario, a set of inputs that was internally consistent and plausible.

EPA started with a flow equal to a waste quantity corresponding to central-tendency and high-end percentiles from the BRS survey data and then sized the units accordingly, using data from the other data sources. This approach reflects the assumption that the exempted waste is the only waste managed in the modeled unit; if other wastes were co-managed, the flow through the unit would be greater than the waste quantity of the exempted waste stream, and the unit would be commensurately larger. The flows from the BRS data, even at the high end of the distribution, are relatively small flows from the perspective of wastewater treatment. Thus, they may be combined with other wastes. However, for nonaerated units, even small waste streams may be managed separately. Therefore, EPA assumed that the potentially exempted waste constitutes all of the flow to the nonaerated units modeled.

Starting with flow, EPA characterized the units using the following steps:

1. **Flow.** EPA chose a flow based on the facility-level waste quantity data from the BRS, using the median for a central-tendency value and the 90th percentile for a high-end value.

2. **Volume.** Using the unweighted SIS data, EPA selected a subset of about 10 impoundments with flows similar to the flows selected in Step 1 for central tendency and high end. Using those impoundments, EPA identified a range of volumes associated with the flow; EPA used the central volume when setting volume to a central-tendency value and the lowest volume when setting volume to a high-end value. EPA took the same approach with the tanks data to select corresponding volumes for tanks.

3. **Depth and Area.** EPA performed a regression to relate area to volume for the SIS data. A similar regression relating depth to volume had already been done with the tanks data for the Air Characteristic Study. EPA used these regressions to estimate a reasonable depth or area for the selected volume. EPA calculated the remaining parameter (area or depth) by dividing volume by depth or area.

4. **Length, Width, or Diameter.** For impoundments, EPA calculated length and width from area by assuming the unit is square. For tanks, EPA calculated diameter from area by assuming the tank is circular.

To set values for the solids diversion parameters for WATER9, EPA used data on solids removal efficiencies and the percentage of diverted sludge that is solids from the SIS survey and calculated the inputs needed for WATER9 from these.

A.2.2.2 Aerated treatment train. Like the nonaerated units, many of the inputs to WATER9 for the aerated treatment train are interrelated. In the case of the aerated treatment train, there is also the added complexity that such treatment trains are rarely sized for a waste stream as small as even the 90th percentile F002/F005 waste stream from the BRS data. The presence of an aerator in the activated sludge unit, for example, places certain limitations on the volume of the unit. Similarly, flows and residence times must be sufficient to maintain the biomass in the activated sludge unit—there must be enough chemical mass as food to feed the biomass or it will die off.

The aerated treatment train units were sized by taking the 50th and 90th percentile flows from the BRS data as a starting point, as was done for nonaerated units. Then, using typical ranges of retention time for activated sludge systems, EPA selected a central-tendency residence time and a high-end residence time. Using the flow and the residence time for a particular scenario, the capacities of the three units (primary clarifier, activated sludge unit, and secondary clarifier) were estimated. The capacities consider the influent flow (from the BRS data), as well as recycle flow from the secondary clarifier to the activated sludge unit.

In sizing the units, EPA determined that the central-tendency flow from the BRS data resulted in unit capacities that were too small to be feasible given good engineering design principles. Therefore, for central-tendency flow, EPA used the smallest flow that resulted in feasible unit capacities. That flow is about the 75th percentile of the BRS data.

It should be noted that the units sized for both 75th percentile flow and 90th percentile flow are still extremely small and are not likely to be typical of actual treatment systems of this type. These systems are small enough that operating such a system would require feeding the biomass because there would be insufficient chemical mass to maintain optimal biomass levels for biodegradation. Real systems are likely to be considerably larger and combine smaller waste streams into one large flow. However, WATER9 is not highly sensitive to the unit capacity and flow for aerated treatment trains designed for biodegradation and aeration-assisted volatilization. These loss processes are much more dependent on residence time. Since the residence times used reflect typical to low-end values (low residence times result in less loss, so greater effluent and sludge concentration), the risk results should be similar or slightly higher than what would be seen if a waste stream with the same concentration were modeled in larger units. Dilution of these wastes with other larger waste streams not containing these chemicals (or containing them at lower concentrations) would have a much greater impact on risk.

Attachment A.2 provides all the WATER9 input values used for each scenario for nonaerated units and the aerated treatment train.

A.2.3 Waste Characteristics

EPA set all waste characteristics to weighted central-tendency values from the SIS survey data. The median active biomass value from the SIS survey data was 0, which is a reasonable value for nonaerated units. Table A-2 presents the waste properties used.

Table A-2. Waste Properties Used in WATER9 Modeling

Parameter	Units	Nonaerated		Aerated Treatment Train	
		Value	Source	Value	Source
Solids	ppmw	141	SIS survey (median)	200	best professional judgment
Oil	ppmw	0	SIS survey (median)	1	best professional judgment
Temperature	C	24.52	Hartford, CT	30	best professional judgment

A.2.4 Physical-Chemical Properties

Some of the WATER9 chemical property default values were updated using the Superfund Chemical Data Matrix (SCDM) (U.S. EPA, 1997). Table A-3 presents the physical-chemical property values used and their source (SCDM or WATER9 database).

Table A-3. Physical-Chemical Properties Used in WATER9

Parameter	Units	Value			Source
		Benzene	2-Ethoxyethanol	1,1,2-Trichloroethane	
Density	g/cm^3	0.88	0.93	1.4	SCDM
Molecular weight	g/mol	78	90	133	SCDM
Diffusivity in water	cm^2/s	1E-5	9.8E-6	1E-5	WATER9
Diffusivity in air	cm^2/s	0.0895	0.082	0.067	WATER9
Vapor pressure	mmHg	95	5.3	23	SCDM
Henry's law constant	$atm\text{-}m^3/m$	5.55E-3	1.23E-7	9.1E-4	SCDM
Vapor pressure temperature coefficient A	unitless	6.9	7.9	7.2	WATER9
Vapor pressure temperature coefficient B	unitless	1,200	1,800	1,500	WATER9
Vapor pressure temperature coefficient C	unitless	220	230	230	WATER9

(continued)

Table A-3. (continued)

Parameter	Units	Value			Source
		Benzene	2-Ethoxyethanol	1,1,2-Trichloroethane	
First-order biorate constant	l/g-hr	1.4	1	0.74	WATER9
Zero-order biorate constant	mg/g-hr	19	20	3.5	WATER9
Log octanol water coefficient (K_{ow})	unitless	2.13	-0.1	2	SCDM
Solubility	mg/L	1,750	1,000,000	4,400	SCDM

A.4 Fate and Transport Inputs

The groundwater DAFs are all for a no-liner scenario. They vary by duration and percentile from the distribution of DAFs. The 50th percentile values were used for central tendency and the 90th percentile DAFs for high end. The duration was chosen to match the exposure duration. Table A-4 shows the DAFs used for surface impoundments, and Table A-5 shows them for landfills. Because 2-ethoxyethanol is a noncarcinogen, calculations for 2-ethoxyethanol are not affected by changes in exposure duration. Therefore, only the 9-year duration is shown for 2-ethoxyethanol.

Table A-4. IWEM Tier I DAFs for Surface Impoundments

Percentile	Benzene		2-Ethoxyethanol	1,1,2-Trichloroethane	
	Duration				
	9-year	30-year	9-year	9-year	30-year
50th	12.5	14.9	12.3	14	16.9
90th	1.4	1.6	1.4	1.4	1.6

Table A-5. IWEM Tier I DAFs for Landfills

Percentile	Benzene		2-Ethoxyethanol	1,1,2-Trichloroethane	
	Duration				
	9-year	30-year	9-year	9-year	30-year
50th	93.5	93.5	95.5	127	127
90th	2.2	2.2	2.2	2.5	2.5

A.5 Exposure Factors

For central-tendency exposure scenarios, exposure duration was set to 9 years. For high-end exposure scenarios, exposure duration was set to 30 years. All other exposure factors are the defaults used in IWEM.

A.6 Toxicity

Attachment A.3 summarizes how health benchmarks were set for IWEM. Table A-6 summarizes the health benchmarks for the three chemicals considered in this assessment.

Table A-6. Health Benchmarks Used in Groundwater Assessment

Chemical	Cancer		Noncancer	
	Ingestion CSF (per mg/kg-d)	Inhalation CSF (per mg/kg-d)	RfD (mg/kg-d)	RfC (mg/m^3)
Benzene				
Central tendency	3.5E-2	5.0E-6	not used	not used
High end	5.5E-2	7.8E-6	not used	not used
2-Ethoxyethanol	NA	NA	0.4	0.2
1,1,2-Trichloroethane	5.7E-2	5.6E-2	not used	not used

A.7 References

RTI. 2001. Risk Assessment Technical Background Document for the Paints and Coatings Hazardous Waste Listing Determination. Submitted to EPA Office of Solid Waste, Washington, DC. http://www.epa.gov/epaoswer/hazwaste/id/paint/ (section 1-2.pdf; section 3-4.pdf; section 5-6.pdf; and section 7-10.pdf).

U.S. EPA (Environmental Protection Agency). 1987. 1986 National Survey of Hazardous Waste, Storage, Disposal, and Recycling Facilities Database.

U.S. EPA (Environmental Protection Agency). 1996. Superfund Chemical Data Matrix (SCDM). Office of Emergency and Remedial Response. Web site at http://www.epa.gov/oerrpage/superfund/resources/scdm/index.htm. June.

U.S. EPA (Environmental Protection Agency). 2001. Industrial Surface Impoundments in the United States. Office of Solid Waste, Washington, DC. EPA530-R-01-005. March.

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Attachment A-1

Description of HBN Development Methodology Used for IWEM

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MEMORANDUM

Date: August 9, 2001

To: Ann Johnson, EPA

From: Susan N. Wolf, Pam Birak, Jessica Lin, and Robert S. Truesdale, RTI

Subject: Description of HBN development methodology used for IWEM

Two Toxicity Reference Levels (TRLs) are included in the Industrial Waste Evaluation Model (IWEM) software: Maximum Contaminant Levels (MCLs), which are available for some waste constituents, and Health-Based Numbers (HBNs), which are available for all waste constituents (including waste constituent daughter products). This memorandum describes the methodology used to develop HBNs for constituents that cause cancer and constituents that produce noncancer health effects.

All constituents currently included in the IWEM software have an ingestion HBN. In IWEM, an ingestion HBN is the maximum concentration of the constituent in groundwater that is not expected to cause adverse health effects in most individuals who drink the groundwater. For organic constituents and mercury, IWEM also uses inhalation HBNs, which are the maximum concentrations of a constituent in groundwater that are not expected to cause adverse health effects in most adults who inhale the constituent while showering. To calculate HBNs, we only consider parameters that describe a constituent's health effects and an individual's (receptor's) exposure to the constituent from drinking or showering. In contrast, the MCL includes consideration of additional factors, such as the cost of treatment, and does not consider the inhalation exposure route.

The sections below provide our methodology for calculating the cancer and noncancer HBNs for ingestion and inhalation of the contituents in IWEM. The target risk used to calculate the HBN for carcinogens is 1×10^{-6} (unitless). The target hazard quotient used to calculate the HBN for noncarcinogens is 1.0 (unitless). These targets are used to calculate independent HBNs for inhalation and ingestion. IWEM does not combine exposure from showering and drinking, but considers these routes of exposure separately to ensure use of the lowest, or most protective, HBN for a particular chemical.

1.0 Ingestion HBNs

The IWEM ingestion HBNs are calculated using equations based on the U.S. Environmental Protection Agency's (EPA's) *Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual* (U.S. EPA, 1991). These equations and inputs

differ for cancer-causing chemicals and chemicals that have adverse health effects other than cancer. The primary differences result from cancer toxicity criteria's being based on an average daily dose over a lifetime, while noncancer health benchmarks use less-than-lifetime estimates of exposure.

1.1 Ingestion HBNs for Constituents That Cause Cancer

The equation for calculating ingestion HBNs for carcinogens uses the cancer slope factor (CSF) exposure variables to determine the highest concentration of the carcinogen in drinking water that will not exceed the target risk. Because the CSF is based on an average day's exposure over a lifetime, the equation also requires estimates of how many days per year a person is exposed (exposure frequency), how many years this exposure continues (exposure duration), and the average amount of water a person drinks every day (intake rate). Duration of exposure is critical because the CSF is based on the lifetime average daily dose. Therefore, we average the total dose received over an average person's lifetime, where the average person's lifetime is the averaging time for the exposure calculation.

$$C\_INGEST\_HBN = \frac{TR \bullet AT \bullet 365}{CSFo \bullet EF \bullet ED \bullet CRw}$$

where

C_INGEST_HBN	=	carcinogenic risk HBN for water due to ingestion (mg/L)
TR	=	target risk for carcinogens = 1×10^{-6}
CSFo	=	oral cancer slope factor $(mg/kg\text{-}d)^{-1}$
AT	=	averaging time (yr) = 70 yrs
EF	=	exposure frequency (d/yr) = 350 d/yr
CRw	=	intake rate of water (L/kg/d)
ED	=	exposure duration (yr)
365	=	conversion factor (d/yr).

The sources for the exposure parameter values used to calculate the cancer HBNs are summarized in Table 1-1. To be protective of exposures to carcinogens in a residential setting, EPA focuses on exposures to individuals who may live in the same residence for a long period of time (i.e., an exposure duration of 30 years, the 95th percentile for population mobility).

Table 1-1. Exposure Parameter Values for Carcinogens

Exposure Parameter	Value	Units	Source
Drinking Water Intake Rate	25.2	mL/kg/d	The value is a time-weighted average of mean drinking water intake rates for adults aged 0 to 29 years. Table 3-7 of the *Exposure Factors Handbook* (U.S. EPA, 1997a)
Exposure Frequency	350	d/yr	The exposure frequency is the number of days per year that an individual is exposed. A value of 350 days per year considers that an individual is away from home for 2 weeks per year. *Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual* (U.S. EPA, 1991)
Exposure Duration	30	yr	The exposure duration is the number of years that an individual is exposed. Thirty years is the 95th percentile value for population mobility (exposure duration). Table 15-176 of the *Exposure Factors Handbook* (U.S. EPA, 1997b)
Averaging Time	70	yr	*Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual* (U.S. EPA, 1991)

1.2 Ingestion HBNs for Constituents that Cause Noncancer Health Effects

To develop ingestion HBNs for constituents that cause health effects other than cancer, we used an equation that determines the maximum concentration that will not exceed the target hazard quotient. The equation uses the reference dose, which is the maximum average daily dose that will not cause adverse health effects, and requires estimates of exposure frequency and water intake rate.

$$NC\_INGEST\_HBN = \frac{THI \bullet RfD \bullet 365}{EF \bullet CRw}$$

where

NC_INGEST_HBN	=	noncarcinogenic risk HBN for water (mg/L)
THI	=	target hazard index for noncarcinogens = 1
RfD	=	reference dose (mg/kg-d)
EF	=	exposure frequency (d/yr) = 350 d/yr
CRw	=	intake rate of water for a child aged 1 to 6 yrs (L/kg/d)
365	=	conversion factor (d/yr).

The sources for the exposure parameter values used to calculate the noncancer HBN are summarized in Table 1-2. Because toxicity criteria for noncarcinogens are based on less-than-lifetime exposures, and to be protective of toxic effects to children, the equation uses a drinking water intake rate that is appropriate for children under 6 years old.

Table 1-2. Exposure Parameter Values for Noncancer Health Effects

Exposure Parameter	Value	Units	Source
Drinking Water Intake Rate	42.6	mL/kg/d	The value is a time-weighted average of mean drinking water intake rates for children aged 0 to 6 years. Table 3-7 of the *Exposure Factors Handbook* (U.S. EPA, 1997a)
Exposure Frequency	350	d/yr	The exposure frequency is the number of days per year that an individual is exposed. A value of 350 days per year considers that an individual is away from home for 2 weeks per year. *Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual* (U.S. EPA, 1991)

2.0 Inhalation HBN Methodology

In IWEM, the inhalation HBN is the maximum concentration of a constituent in groundwater that is not expected to cause adverse health effects in most adults who inhale the constituent as a result of activities associated with showering (we assume that children take baths; consequently, we do not evaluate children's shower-related exposure). The inhalation HBN is the groundwater concentration that results in a target risk of 1×10^{-6} for carcinogens or a

target hazard quotient of 1 for noncarcinogens. We only calculated inhalation HBNs for constituents that (1) volatilize (e.g., mercury and organic constituents) and (2) have an inhalation health benchmark available (e.g., reference concentrations [RfC], inhalation unit risk factors [URF], and/or inhalation cancer slope factors [CSFi]). Inhalation HBNs were not calculated for airborne metal particles because we do not expect these to be produced by a shower.

We developed the inhalation HBNs in two basic steps. First, Section 2.1 describes how we used a shower model to calculate the average concentration of a waste constituent in air that an adult will be exposed to both during showering and during time spent in the shower stall and/or bathroom after showering. (The HBNs do not reflect inhalation exposure to groundwater that results from other household uses of water.) Because the relationship between groundwater concentration and risk (or hazard quotient) is linear, we used a single unit groundwater concentration (e.g., 1 mg/L) that was within the solubility limits of the constituent so that the model would calculate a unit average shower air concentration. To reflect average daily dose, the model adjusted this unit shower air concentration and outputs a unit average daily indoor air concentration for the second step of the analysis.

Second, we used this unit average indoor air concentration in air to calculate the HBN. The HBN equations first calculate the risk or hazard quotient associated with the unit air concentrations from the shower model, and then use ratios to determine the groundwater concentration (or HBN) associated with the target risk level or target hazard quotient. Section 2.2 describes the application of the HBN equations for cancer-causing chemicals and for chemicals with non-cancer health effects.

2.1 Calculation of Exposure Concentrations from Showering

Individuals may be exposed to waste constituents through inhalation of vapor-phase emissions from groundwater. Such exposure may occur during the time spent in the shower while showering, in the shower stall after showering, and in the bathroom after showering. To evaluate these exposures, EPA used a shower model to calculate the average constituent concentration in the shower stall and bathroom air. This section describes this model and assumptions (Section 2.1.1) along with uncertainties and limitations associated with its use (Section 2.1.2).

A primary assumption of this evaluation is that the gas-phase concentration of a constituent results solely from showering activity. Previous versions of the shower model included emissions due to other household uses of water and risks due to inhalation for time spent in the remainder of the house. However, the risk from inhalation exposures in the remainder of the house has been shown to be several orders of magnitude lower than the risk from inhalation exposures in the bathroom and during showering (EPA, 1997d). Given the low risk due to exposure from the remainder of the house and the difficulty in collecting the input data needed to estimate household chemical concentrations from other sources, the current version of the shower model has been simplified to focus on the greatest sources of exposure and risk due to use of contaminated water.

2.1.1 Shower Model

The shower model estimates the change in the shower constituent air concentrations over time as a function of the mass of constituent transferred from the shower water to shower vapors. After calculating the predicted vapor-phase constituent concentration in the shower stall and bathroom during showering, the model calculates an average daily indoor air concentration using volumetric air exchange rates between the shower stall, bathroom, and house. The shower model is based on differential equations presented in McKone (1987) and Little (1992). Memo Attachment A provides details on these equations and explains how we implemented them in the model. Tables A-1 to A-11 (in Memo Attachment A) present the equations, and Table A-12 (in Memo Attachment A) provides the model parameters for exposure (e.g., exposure time, shower properties).

The model's calculations of mass transfer between the liquid and vapor phases of the constituent in the shower, and subsequent air transfer between the shower stall and bathroom depend on both physical parameters (shower properties) and chemical-specific properties. With respect to chemical-specific properties, a constituent's ability to transfer mass from the liquid phase to gas phase is characterized by its diffusivity, or how well it mixes with other gases. Diffusion coefficients in air and water quantify diffusivity for each constituent, which depends on the constituent's density and molecular weight. Transfer from the shower water to air is controlled by the air pressure in the shower stall. We used Henry's law to quantify the amount of constituent dissolved in the shower water (equation in Table A-3 of Memo Attachment A). Henry's law states that the amount of a gas dissolved in solution is directly proportional to the pressure of the gas above the solution. Once a constituent's diffusion coefficients in air and water and its Henry's law constant coefficient were known, an overall mass transfer coefficient was calculated to quantify the constituent's ability to volatilize from the shower water into the air (equation in Table A-5 of Memo Attachment A).

The physical properties of the shower also affect constituent air concentrations. There are macro-level parameters, such as the volume of the shower stall, the water flow rate, and the height of the nozzle, which limit the length of time the constituent is in the shower stall and the amount of it that may accumulate in the shower air. These macro-level physical parameters were set to standard values, based on available literature (see Table 2-1). These shower parameters provide a cap on the maximum possible constituent concentration that may accumulate in the shower stall, and they are required to calculate equilibrium constituent concentrations between the water and air during shower time (equations in Table A-6 of Memo Attachment A).

On a smaller scale, the fraction of constituent emitted by a water droplet into the shower air depends upon the level of gas-phase saturation in the shower stall and a dimensionless mass transfer coefficient (equation in Table A-7 of Memo Attachment A). Calculation of the dimensionless mass transfer coefficient uses micro-level droplet properties, such as droplet diameter and velocity, and some macro-level shower properties discussed above to quantify the length of time a constituent is in contact with the surrounding air and the amount that may volatilize (surface area of the droplet) (equation in Table A-4 of Memo Attachment A). The droplet's diameter (0.098 cm) and velocity (400 cm/s) were set to constant values that correlated well with existing data (Table 2-1).

Table 2-1. Shower Model Input Parameters

Input Parameter	Description	Value	Units	Reference	Comment
ShowerStallTime	Time in shower stall after showering	5	min	U.S. EPA, 1997c	Table 15-23. 50th percentile overall
T_bathroom	Time spent in bathroom, not in shower	5	min	U.S. EPA, 1997c	Table 15-32. 50th percentile overall
ShowerTime	Shower time, 50th percentile	15	min	U.S. EPA, 1997c	Table 15-21. 50th percentile overall
Vb	Volume of the bathroom	10	m^3	McKone, T., 1987	
Vs	Volume of shower	2	m^3	McKone, T., 1987	
NozHeight	Height of shower head	1.8	m	Little, J., 1992	Selected based on the maximum height reported in Table 1, a summary of five studies.
Qsb	Volumetric exchange rate between the shower and the bathroom	100	L/min	RTI-derived value	Estimated from the volume and flow rate in McKone (1987) such that the exchange rate equals the volume divided by the residence time (e.g., 2000L/20 min).
ShowerRate	Rate of water flow from shower head	10	L/min	RTI-derived value	Value obtained by averaging the flow rates reported in five studies in Table 1 of Little (1992) (QL) = 10.08 L/min.
DropVel	Terminal velocity of water drop	400	cm/s	RTI-derived value	Selected value by correlating to existing data.
DropDiam	Diameter of shower water drop	0.098	cm	RTI-derived value	Estimated as a function of terminal velocity<=600cm/sec (Coburn, 1996).
Qbh	Volumetric exchange rate between the bathroom and the house	300	L/min	RTI-derived value	Estimated from the volume and flow rate in McKone (1987) such that the exchange rate equals the volume divided by the residence time (e.g., 10,000L/30 min).
Cin	Constituent concentration in incoming water	0.001	mg/L	NA	Unit concentration selected.

After calculating the fraction of constituent that can be emitted from a droplet, the shower model calculates the potential amount of constituent mass that may be emitted into the air during 0.2-minute time steps for the duration of the showering time. The mass emitted during a time step is limited by the fraction that can be emitted and the existing gas-phase constituent concentration in the shower stall at the beginning of the time step. We calculate this incremental mass using the physical parameters of the shower in conjunction with constituent-specific properties to estimate how much constituent may accumulate in the shower air (equation in Table A-6 of Memo Attachment A).

Because of air flow between the shower stall and bathroom, the actual gas-phase constituent concentration in the shower is less than the potential amount calculated above. The volumetric exchange rates between the shower stall and bathroom and the bathroom and rest of the house were assigned constant values derived from McKone (1987) (Table 2-1). These two parameters quantify the dilution of constituent concentration in the shower air. The shower model uses these two loss components to calculate the actual constituent concentration in the shower stall and in the bathroom at the end of each time step (equations in Tables A-9 and A-10 of Memo Attachment A).

To calculate average daily indoor air concentrations, values for exposure time were taken from the *Exposure Factors Handbook* (EPA, 1997a). We selected the 50th percentile for adults' time spent taking a shower, time spent in the shower stall after showering, and time spent in the bathroom after showering (Table 2-1). The shower model calculates constituent concentrations in the shower stall and bathroom for each time step until the end of the time spent in the shower and bathroom, and then averages constituent concentrations for the two compartments. The model then calculates the daily indoor constituent concentration by averaging these concentrations over the length of an entire day (equation in Table A-11 of Memo Attachment A), assuming that there is no additional inhalation exposure to the constituent during the day (i.e., that the gas-phase constituent concentration in the house is negligible).

2.1.2 Shower Model Uncertainties and Limitations

A primary limitation of the shower model is that the gas-phase concentration of a constituent in the house results only from shower-related activities. The model does not include other household uses of water (e.g., toilet use) in calculating average indoor concentrations. However, the risk of inhalation exposure from other water use activities has been demonstrated to be several magnitudes lower than the exposure risk from showering (EPA, 1997d). In addition, there is also large uncertainty in estimating other household-activity chemical concentrations. To quantify the inhalation exposure risk for the entire house, the model would require an estimate of the air exchange rate between the house and outdoor air, exposure time in the house, and the amount of nonshower water usage. Given the uncertainties in these input parameters and the low risk due to exposure from the remainder of the house, the shower model focuses only on the greatest source of exposure and risk due to use of contaminated water.

The input parameter values are another source of uncertainty for the shower model. In selecting values for the shower properties (shower and bathroom volume, nozzle height, and

flow rate), we used in most cases mid-range values that were reported in the literature. Though setting the shower parameters to constants does not capture possible variability in these variables, the results using these fixed values compare favorably to experimental data for numerous organic compounds of varying volatility (Coburn, 1996). The droplet properties (diameter and velocity) are also constants, but their values were selected based on correlation to existing data, resulting in less uncertainty. The largest uncertainty is likely in the volumetric exchange rates used between the shower and bathroom and the bathroom and the rest of house. These values, 300 L/min for the exchange rate between the bathroom and the house, and 100 L/min for the exchange rate between the shower and the bathroom, were derived from McKone (1987). The range of values reported in a five-study summary (Little, 1992), however, was 35 to 460 L/min for exchange between the shower and the bathroom and 38 to 480 L/min for exchange between the bathroom and the rest of the house, making these the most uncertain variables among the shower model inputs.

2.2 Calculating Inhalation HBNs

To calculate HBNs, we selected a unit groundwater concentration (usually 1 mg/L) within the solubility limits of each constituent and ran the shower model using that concentration to calculate a unit average daily indoor air concentration. We used this unit air concentration to calculate a corresponding unit risk (for cancer-causing chemicals) or unit hazard quotient (for constituents with noncancer health effects). Because there is a linear relationship between groundwater concentration and risk, we could use simple ratios to adjust the unit groundwater concentrations to the groundwater concentration corresponding to the target risk or target hazard quotient (i.e., the inhalation HBN). Section 2.2.1 describes this process for carcinogens while Section 2.2.2 discusses the approach we used for noncarcinogens. As a final step, we checked every inhalation HBN to ensure that it did not exceed the constituent's solubility, as described in Section 2.2.3.

2.2.1 Inhalation HBNs for Carcinogens

To calculate the inhalation HBN for carcinogens, we first calculate the average daily dose (ADD) from inhalation due to exposure to contaminated groundwater during showering. The ADD is calculated from the unit air concentration output by the shower model, as follows:

$$ADD = \frac{Cair\_indoor \bullet IR}{BW}$$

where

ADD	=	average daily dose (mg/kg-d) at the unit groundwater concentration
Cair_indoor	=	average air concentration over a day (mg/m^3) (calculated from the unit groundwater concentration using the shower model)
IR	=	inhalation rate (m^3/d)

BW	=	body weight (kg).

We then calculated the risk at the modeled unit groundwater concentration from the ADD, as shown below:

$$Risk\_modeled = \frac{(ED \bullet EF)}{(AT \bullet 365)} \bullet CSFi \bullet ADD$$

where

Risk_modeled	=	risk resulting from groundwater concentration modeled
ED	=	exposure duration (yr) = 30 yr
EF	=	exposure frequency (d/yr) = 350 d/yr
AT	=	averaging time (yr) = 70 yr
CSFi	=	inhalation cancer slope factor $(mg/kg\text{-}d)^{-1}$
ADD	=	average daily dose (mg/kg-d) at the unit groundwater concentration
365	=	conversion factor (d/yr).

We then derived the target groundwater concentration (i.e., the inhalation HBN) by adjusting the modeled unit groundwater concentration using the simple ratio of target risk to the modeled risk:

$$HBN = \frac{Risk\_T \bullet C\_GW\_modeled}{Risk\_modeled}$$

where

HBN	=	concentration in groundwater resulting in target risk (µg/L)
C_GW_modeled	=	unit concentration in groundwater used in shower model (µg/L)
Risk_T	=	target risk for carcinogens = 1×10^{-6}
Risk_modeled	=	risk resulting from groundwater concentration modeled.

This equation assumes that the relationship between groundwater concentration and risk is linear, which we confirmed by running the shower model using the target groundwater concentration for several constituents and comparing the results to the target risk level.

The inhalation HBNs for cancer-causing chemicals were based on adult exposure parameters. The sources for the exposure parameter values used in the equations above are summarized in Table 2-2.

Table 2-2. Exposure Parameter Values

Exposure Parameter	Value	Units	Source
Inhalation Rate	13.25	m^3/d	The value corresponds to the mean inhalation rates for adults aged 19 to 65+. The value was calculated by averaging the daily mean inhalation rates for females (11.3 m^3/d) and males (15.2 m^3/d). Table 5-23 of the *Exposure Factors Handbook* (U.S. EPA, 1997a)
Body Weight	71.8	kg	The value corresponds to the mean body weight of 18- to 75-year-old men and women. Tables 7-2 and 7-11 of the *Exposure Factors Handbook* (U.S. EPA, 1997a)
Exposure Frequency	350	d/yr	The exposure frequency is the number of days per year that an individual is exposed. A value of 350 days per year considers that an individual is away from home for 2 weeks per year. *Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual* (U.S. EPA, 1991)
Exposure Duration	30	yr	The exposure duration is the number of years that an individual is exposed. Thirty years is the 95th percentile value for population mobility (exposure duration). Table 15-176 of the *Exposure Factors Handbook* (U.S. EPA, 1997b)
Averaging Time	70	yr	*Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual* (U.S. EPA, 1991)

2.2.1 Inhalation HBNs for Noncarcinogens

Calculating inhalation HBNs for noncarcinogens is simpler than calculating them for carcinogens because the toxicity criterion (RfC) is expressed as a concentration in air. The HBN

is calculated by first determining the hazard quotient resulting from the unit air concentration output by the shower model:

$$HQ\_modeled = \frac{Cair\_indoor}{RfC}$$

where

HQ_modeled	=	hazard quotient resulting from the groundwater concentration modeled
Cair_indoor	=	average air concentration over a day (mg/m^3) (calculated from the unit groundwater concentration using the shower model)
RfC	=	reference concentration (mg/m^3).

We then derived the target groundwater concentration (i.e., the inhalation HBN) by adjusting the modeled unit groundwater concentration using the simple ratio of target hazard quotient to the modeled hazard quotient:

$$HBN = \frac{THQ \bullet C\_GW\_modeled}{HQ\_modeled}$$

where

HBN	=	concentration in groundwater resulting in target hazard quotient (µg/L)
C_GW_modeled	=	unit concentration in groundwater used in shower model (µg/L)
THQ	=	target hazard quotient for noncarcinogens = 1
HQ_modeled	=	hazard quotient resulting from groundwater concentration modeled.

2.2.3 Solubility Check

After calculation, we checked each HBN to ensure that it did not exceed the solubility of the chemical in water (see Memo Attachment B for the aqueous solubilities used for this check). This check was necessary because above the solubility limit, the water is saturated with the chemical, and any additional chemical is present in a free, separate phase (pure liquid or solid). Above saturation, Henry's law (a basic principle of the shower volatilization model) does not apply, and the emission flux from water to air reaches a plateau. In other words, volatile emissions will not increase above this level no matter how much chemical is added to the water (U.S. EPA, 1996). Because of this fact, a calculated HBN above solubility indicates that a constituent does not pose a significant inhalation risk, and IWEM does not include an inhalation HBN for that constituent. In these cases, IWEM will evaluate the constituent based on its ingestion risk alone.

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Memo Attachment A

Shower Algorithms

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Table A-1. Total time spent in shower and bathroom

Shower

$$BSResTime = ShowerTime + ShowerStallTime + T\_bathroom$$

Name	Description	Value
BSResTime	Total time spent in shower and bathroom (min)	Calculated above
ShowerTime	Duration of shower (min)	Provided in Table A-12
ShowerStallTime	Time in shower stall after showering (min)	Provided in Table A-12
T_bathroom	Time spent in bathroom, not in shower (min)	Provided in Table A-12

This equation calculates the total time that a receptor is exposed to vapors.

Table A-2. Total time spent in shower stall

Shower

$$ShowerResTime = ShowerStallTime + ShowerTime$$

Name	Description	Value
ShowerResTime	Total time spent in shower stall (min)	Calculated above
ShowerStallTime	Time in shower stall after showering (min)	Provided in Table A-12
ShowerTime	Duration of shower (min)	Provided in Table A-12

This equation calculates the total time that a receptor is exposed to vapors in the shower stall.

Table A-3. Dimensionless Henry's law constant

Shower

$$Hprime = HLCcoef \times HLC$$

$$HLCcoef = \frac{1}{R \times Temp}$$

Name	Description	Value
Hprime	Dimensionless Henry's law constant (dimensionless)	Calculated above
HLCcoef	Coefficient to Henry's law constant (dimensionless)	Calculated above
HLC	Henry's law constant (atm-m^3/mol)	Chemical-specific
R	Ideal Gas constant (atm-m^3/K-Mol)	0.00008206
Temp	Temperature (K)	298

This equation calculates the dimensionless form of Henry's law constant.

Table A-4. Dimensionless overall mass transfer coefficient

Shower

$$N = Kol \times AVRatio \times DropResTime$$

$$AVRatio = \frac{6}{DropDiam}$$

$$DropResTime = \frac{NozHeight \times 100}{DropVel}$$

Name	Description	Value
N	Dimensionless overall mass transfer coefficient (dimensionless)	Calculated above
AVRatio	Area-to-volume ratio for a sphere (cm^2/cm^3)	Calculated above
Kol	Overall mass transfer coefficient (cm/s)	Calculated in Table A-5
DropResTime	Residence time for falling drops (s)	Calculated above
DropDiam	Drop diameter (cm)	Provided in Table A-12
NozHeight	Nozzle height (m)	Provided in Table A-12
DropVel	Drop terminal velocity (cm/s)	Provided in Table A-12
100	Conversion factor (cm/m)	Conversion factor

This equation calculates the dimensionless overall mass transfer coefficient. The above equation is based on Little (1992a), which provides the equation as N = Kol × A/Q1 where A is surface area and Q1 is flow in volume per time.

Table A-5. Overall mass transfer coefficient

Shower

$$Kol = \beta \times \left(\frac{2.5}{Dw^{2/3}} + \frac{1}{Da^{2/3} \times Hprime} \right)^{-1}$$

Name	Description	Value
Kol	Overall mass transfer coefficient (cm/s)	Calculated above
beta	Proportionality constant (cm-s^-1/3)	216
Dw	Diffusion coefficient in water (cm^2/s)	Chemical-specific
Da	Diffusion coefficient in air (cm^2/s)	Chemical-specific
Hprime	Dimensionless Henry's law constant (dimensionless)	Calculated in Table A-3

This equation calculates the overall mass transfer coefficient. The above equation corresponds to Equation 17 in McKone (1987) and was modified to use the dimensionless Henry's law constant. The value for beta was derived based on data for benzene and verified for chemicals of varying volatility (Coburn, 1996).

Table A-6. Contaminant mass emitted in the shower for a given time step

Shower

For Et > Emax,

$$Es = Emax$$

For Et $\leq$ Emax,

$$Es = Et$$

Where,

$$Et = Cin \times ShowerRate \times ts \times fem$$

$$Emax = \left(y_{eq} - y_{s,t}\right) \times Vs \times 1000$$

Name	Description	Value
Es	Contaminant mass emitted in the shower for a given time step (mg)	Calculated above
Emax	Maximum possible mass of constituent emitted from shower during time step (mg)	Calculated above
Et	Potential mass of constituent emitted from shower during time step (mg)	Calculated above
yeq	Gas-phase constituent concentration in equilibrium between water and air (mg/L)	Hprime x Cin
ys, t	Gas-phase constituent concentration in the shower at the beginning of time step (mg/L)	Calculated from last time step
Vs	Volume of shower (m^3)	Provided in Table A-12
Cin	Liquid-phase constituent concentration in the incoming water (mg/L)	Provided in Table A-12
ShowerRate	Rate of flow from showerhead (L/min)	Provided in Table A-12
ts	Time step (min)	0.2
fem	Fraction of constituent emitted from a droplet (dimensionless)	Calculated in Table A-7
Hprime	Dimensionless Henry's law constant (dimensionless)	Calculated in Table A-3
1000	Conversion factor (L/m^3)	Conversion factor

The above equations are used to determine the mass of contaminant emitted for a given time step. The equilibrium concentration in air (y_eq) is calculated from Equation 1 in Little (1992a). If the mass emitted based on the mass transfer coefficient (Et) is greater than the amount emitted to reach equilibrium (Emax), the mass is set to the amount that results in the air concentration at equilibrium.

Table A-7. Fraction of constituent emitted from a droplet

Shower

$$fem = \left(1 - Fsat\right) \times \left(1 - e^{-N}\right)$$

Name	Description	Value
fem	Fraction of constituent emitted from a droplet (dimensionless)	Calculated above
Fsat	Fraction of gas-phase saturation (dimensionless)	Calculated in Table A-8
N	Dimensionless overall mass transfer coefficient (dimensionless)	Calculated in Table A-4

This equation is used to calculate the fraction of a given chemical emitted from a droplet of water in the shower. The equation is based on Equation 5 in Little (1992a). The above equation is obtained by rearranging the equation in Little given that ys_max/m = Cin and f_sat = ys/ys_max = ys/(m × Cin).

Table A-8. Fraction of gas-phase saturation in shower

Shower

$$Fsat = \frac{y_{s,\,t}}{y_{eq}}$$

Name	Description	Value
Fsat	Fraction of gas-phase saturation in shower (dimensionless)	Calculated above
yeq	Gas-phase contaminant concentration in equilibrium between water and air (mg/L)	Hprime x Cin
ys, t	Current gas-phase contaminant concentration in air (mg/L)	Calculated in Table A-9 (as ys, t+ts for previous time step)
Hprime	Dimensionless Henry's law constant (dimensionless)	Calculated in Table A-3
Cin	Constituent concentration in incoming water (mg/L)	Provided in Table A-12

This equation is used to calculate the fraction of gas phase saturation in shower for each time step. The equilibrium concentration in air (y_eq) is calculated from Equation 1 in Little (1992a).

Table A-9. Gas-phase constituent concentration in the shower at end of time step

Shower

$$y_{s,\,t+ts} = y_{s,\,t} + \frac{\left[E_s - \left(Q_{sb} \times \left(y_{s,\,t} - y_{b,\,t}\right) \times ts\right)\right]}{V_s \times 1000}$$

Name	Description	Value
ys, t+ts	Gas-phase constituent concentration in the shower at end of time step (mg/L)	Calculated above
ys, t	Gas-phase constituent concentration in the shower at the beginning of time step (mg/L)	Calculated from last time step
yb, t	Gas-phase constituent concentration in the bathroom at the beginning of time step (mg/L)	Calculated from last time step
Es	Mass emitted in the shower for a given time step (mg)	Calculated in Table A-6
Qsb	Volumetric exchange rate between the shower and the bathroom (L/min)	Provided in Table A-12
Vs	Volume of shower (m^3)	Provided in Table A-12
ts	Time step (min)	0.2
1000	Conversion factor (L/m^3)	Conversion factor

This equation is used to calculate the gas-phase constituent concentration in the shower at end of time step. The equation is derived from Equation 9 in Little (1992a). Es is set to 0 when the shower is turned off (i.e., at the end of showering) to estimate the reduction in shower stall air concentrations after emissions cease.

Table A-10. Gas-phase constituent concentration in the bathroom at end of time step

Shower

$$y_{b,\,t+ts} = y_{b,\,t} + \frac{\left[\left(Q_{sb} \times \left(y_{s,\,t+ts} - y_{b,\,t}\right) - Q_{bh} \times \left(y_{b,\,t} - y_{h,\,t}\right)\right)\right]}{V_b \times 1000} \times ts$$

Name	Description	Value
yb, t+ts	Gas-phase constituent concentration in the bathroom at end of time step (mg/L)	Calculated above
yb, t	Gas-phase constituent concentration in the bathroom at the beginning of time step (mg/L)	Calculated from last time step
ys, t+ts	Gas-phase constituent concentration in the shower at the end of time step (mg/L)	Calculated in Table A-9
yh, t	Gas-phase constituent concentration in the house at the beginning of time step (mg/L)	Assumed deminimus, zero
Qsb	Volumetric exchange rate between the shower and the bathroom (L/min)	Provided in Table A-12
Qbh	Volumetric exchange rate between the bathroom and the house (L/min)	Provided in Table A-12
Vb	Volume of bathroom (m^3)	Provided in Table A-12
ts	Time step (min)	0.2
1000	Conversion factor (L/m^3)	Conversion factor

This equation is used to calculate the gas-phase constituent concentration in the bathroom at end of time step. The equation is derived from Equation 10 in Little (1992a).

Table A-11. Average daily concentration in indoor air

Shower

$$C_{air\_indoor} = \frac{\left(C_{air\_shower} \times ShowerResTime\right) + \left(C_{air\_bathroom} \times T\_bathroom\right)}{1440}$$

$$C_{air\_shower} = \frac{\sum \left[\left(y_{s,\,t+ts} + y_{s,\,t}\right)/2\right] \times 1000}{n_s}$$

$$C_{air\_bathroom} = \frac{\sum \left[\left(y_{b,\,t+ts} + y_{b,t}\right)/2\right] \times 1000}{n_b}$$

Name	Description	Value
Cair_indoor	Average daily concentration in indoor air (mg/m^3)	Calculated above
Cair_shower	Average concentration in shower (mg/m^3)	Calculated above
Cair_bathroom	Average concentration in bathroom (mg/m^3)	Calculated above
ShowerResTime	Total time spent in shower stall (min)	Calculated in Table A-2
T_bathroom	Time spent in bathroom, not in shower (min)	Provided in Table A-12
ys, t	Gas-phase constituent concentration in the shower at the beginning of time step (mg/L)	Calculated from last time step
ys, t+ts	Gas-phase constituent concentration in the shower at the end of time step (mg/L)	Calculated in Table A-9
yb, t	Gas-phase constituent concentration in the bathroom at the beginning of time step (mg/L)	Calculated from last time step
yb, t+ts	Gas-phase constituent concentration in the bathroom at the end of time step (mg/L)	Calculated in Table A-10
ns	Number of time steps corresponding to time spent in the shower (dimensionless)	Summed in model code
nb	Number of time steps corresponding to time spent in the bathroom (dimensionless)	Summed in model code
1440	Minutes per day (min)	
1000	Conversion factor (L/m^3)	Conversion factor

The above equations are used to calculate the time-weighted average daily indoor air concentration to which a receptor is exposed. The equation assumes that receptors are only exposed to contaminants in the shower and bathroom.

Table A-12. Model parameters for exposure

Name	Description	Value	Reference	Comments
Bathroom properties				
Vb	Volume of the bathroom (m^3)	10	McKone, T., 1987	
Exchange rate				
Qbh	Volumetric exchange rate between the bathroom and the house (L/min)	300	RTI-derived value	Estimated from the volume and flow rate in McKone (1987) such that the exchange rate equals the volume divided by the residence time (i.e., 10,000L/30 min).
Qsb	Volumetric exchange rate between the shower and the bathroom (L/min)	100	RTI-derived value	Estimated from the volume and flow rate in McKone (1987) such that the exchange rate equals the volume divided by the residence time (i.e., 2000L/20 min).
Exposure time				
ShowerStallTime	Time in shower stall after showering (min)	0	NA	Only assessing exposure from time spent showering.
ShowerTime	Shower time, 50th percentile (min)	15	U.S. EPA, 1997	Table 15-21, 50th percentile overall.
T_bathroom	Time spent in bathroom, not in shower (min)	0	NA	Only assessing exposure from time spent showering.
Shower properties				
DropDiam	Diameter of shower water drop (cm)	0.098	RTI-derived value	Estimated as a function of terminal velocity (Coburn, 1996).
DropVel	Terminal velocity of water drop (cm/s)	400	RTI-derived value	Estimated by correlating to existing data (Coburn, 1996).
NozHeight	Height of shower head (cm)	180	Little, J., 1992a	Selected based on values presented in Little.
ShowerRate	Rate of water flow from shower head (L/min)	5.5	RTI-derived value	Calculated based on droplet diameter and nozzle velocity.
Vs	Volume of shower (m^3)	2	McKone, T., 1987	
Groundwater				
Cin	Constituent concentration in incoming water (mg/L)	0.001	NA	Unit concentration selected.

Memo Attachment B

Contaminant-Specific Chemical and Physical Properties

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Memo Attachment B

Contaminant-Specific Chemical and Physical Properties

To calculate inhalation HBNs, the shower model requires input of several chemical-specific properties, including Henry's law constant *(HLC)*, solubility *(Sol)*, and diffusion coefficients in air *(D_a)* and water *(D_w)*. This attachment describes the data sources and methodologies used to collect and develop these properties. Table B-1 (at the end of this attachment) lists by contaminant the chemical-specific properties used to calculate inhalation HBNs, along with the data source for each value.

B.1 Data Collection Procedure

To select data values available from multiple sources, we created a hierarchy of references based on the reliability and availability of data in such sources. Our first choice for data collection and calculations was EPA reports and software. When we could not find data or equations from EPA publications, we consulted highly recognized sources, including chemical information databases on the Internet. These on-line sources are compilations of data that provide the primary references for data values. The specific hierarchy varied among properties as described in subsequent sections.

For dioxins, the preferred data source in all cases was the *Exposure and Human Health Reassessment of 2,3,7,8-Tetrachlorodibenzo-p-Dioxin (TCDD) and Related Compounds, Part 1, Vol. 3* (*Dioxin Reassessment*) (U.S. EPA, 2000). We used the *Mercury Study Report to Congress* (U.S. EPA, 1997a) as the preferred source for mercury properties. If values were unavailable from these sources, we followed the same reference hierarchy that was used for other contaminants.

All data entry for chemical and physical properties was checked by comparing each entry against the original online or hardcopy reference. All property calculation programs were checked using hand calculations to ensure that they were functioning correctly.

B.2 Solubility (Sol)

For solubility *(Sol)* values, we looked for data by searching the following sources in the following order:

1. Superfund Chemical Data Matrix (SCDM) (U.S. EPA, 1997b);
2. CHEMFATE Chemical Search (SRC, 1999);
3. Hazardous Substances Data Bank (HSDB) (U.S. NLM, 2001);
4. ChemFinder (CambridgeSoft Corporation, 2001).

For mercury, we obtained a solubility for elemental mercury from *The Merck Index*: *An Encyclopedia of Chemicals, Drugs, and Biologicals* (Budavari, 1996).

B.3 Henry's Law Constant (HLC)

Collection of Henry's law constant *(HLC)* data proceeded by searching sources in the following order:

1. SCDM;
2. CHEMFATE;
3. HSDB.

When we could not find data from these sources, we calculated HLC using equation 15-8 from Lyman, Reehl, and Rosenblatt (1990):

$$HLC = \frac{P_{vp}}{Sol}$$

where

HLC	=	Henry's law constant (atm-m^3/mole*)*
P_{vp}	=	vapor pressure (atm)
Sol	=	solubility (mol/m^3).

B.4 Diffusion Coefficient in Water (D_w)

For all chemicals, we calculated the diffusion coefficient in water (D_w) by hand because few empirical data are available. The preferred calculation was equation 17-6 from the WATER9 model (U.S. EPA, 2001):

$$D_w = 0.0001518\left(\frac{T + 273.16}{298.16}\right)\left(\frac{MW}{\rho}\right)^{-0.6}$$

where

D_w	=	diffusion coefficient in water (cm^2/s)
T	=	temperature (degrees C)
MW	=	molecular weight (g/g-mol)
ρ	=	density (g/cc).

When we did not know chemical density, we used equation 3.16 from *Process Coefficients and Models for Simulating Toxic Organics and Heavy Metals in Surface (Process Coefficients)* (U.S. EPA, 1987), which only requires molecular weight:

$$Dw = 0.00022 \times MW^{-2/3}$$

where

D_w = diffusion coefficient in water (cm^2/s)
MW = molecular weight (g/mol).

B.5 Diffusion Coefficient in Air (D_a)

All diffusion coefficients in air (D_a) were calculated values because few empirical data are available. Similar to D_w, we first consulted WATER9 and then used U.S. EPA (1987). Equation 17-5 in WATER9 calculates diffusivity in air as follows:

$$D_a = \frac{0.0029(T + 273.16)^{1.5}\sqrt{0.034 + \frac{1}{MW}}\left(1 - 0.000015MW^2\right)}{\left[\left(\frac{MW}{2.5\rho}\right)^{0.333} + 1.8\right]^2}$$

where

D_a = diffusion coefficient in air (cm^2/s)
T = temperature (degrees C)
MW = molecular weight (g/g-mol)
ρ = density (g/cc).

When density was not available, we used equation 3.17 from *Process Coefficients* (U.S. EPA, 1987):

$$Da = 1.9 \times MW^{-2/3}$$

where

D_a = diffusion coefficient in air (cm^2/s)
MW = molecular weight (g/mol).

For dioxins and dibenzofurans, we used an equation from the *Dioxin Reassessment* (U.S. EPA, 2000) to estimate diffusion coefficients from diphenyl's diffusivity:

$$\frac{D_a}{D_b} = \left(\frac{MW_b}{MW_a}\right)^{0.5}$$

where

D_a = diffusion coefficient of constituent in air (cm^2/s)
D_b = diffusion coefficient of diphenyl at 25 degrees C (0.068 cm^2/s)
MW_a = molecular weight of constituent (g/mole)
MW_b = molecular weight of diphenyl (154 g/mole).

Table B-1. Contaminant-specific Chemical and Physical Properties

Contaminant	CASRN	D_a (cm^2/s)	D_w (cm^2/s)	HLC ($atm\text{-}m^3/mol$)	Sol (mg/L)
Acetaldehyde (ethanal)	75-07-0	1.28E-01 e	1.35E-05 e	7.89e-05 a	1.00e+06 a
Acetone (2-propanone)	67-64-1	1.06E-01 e	1.15E-05 e	3.88e-05 a	1.00e+06 a
Acetonitrile (methyl cyanide)	75-05-8	1.34E-01 e	1.41E-05 e	3.46e-05 a	1.00e+06 a
Acrolein	107-02-8	1.12E-01 e	1.22E-05 e	1.22e-04 a	2.13e+05 a
Acrylamide	79-06-1	1.07E-01 e	1.26E-05 e	1.00e-09 a	6.40e+05 a
Acrylic acid (propenoic acid)	79-10-7	1.03E-01 e	1.20E-05 e	1.17e-07 a	1.00e+06 a
Acrylonitrile	107-13-1	1.14E-01 e	1.23E-05 e	1.03e-04 a	7.40e+04 a
Aldrin	309-00-2	2.28E-02 e	5.84E-06 e	1.70e-04 a	1.80e-01 a
Aniline (benzeneamine)	62-53-3	8.30E-02 e	1.01E-05 e	1.90e-06 a	3.60e+04 a
Benz(a)anthracene	56-55-3	5.09E-02 b	5.89E-06 b	3.35e-06 a	9.40e-03 a
Benzene	71-43-2	8.95E-02 e	1.03E-05 e	5.55e-03 a	1.75e+03 a
Benzidine	92-87-5	3.55E-02 e	7.59E-06 e	3.88e-11 a	5.00e+02 a
Benzo(a)pyrene	50-32-8	2.55E-02 e	6.58E-06 e	1.13e-06 a	1.62e-03 a
Benzo(b)fluoranthene	205-99-2	4.76E-02 b	5.51E-06 b	1.11e-04 a	1.50e-03 a
Benzyl chloride	100-44-7	6.34E-02 e	8.81E-06 e	4.15e-04 a	5.25e+02 a
Bis(2-ethylhexyl)phthalate	117-81-7	1.73E-02 e	4.18E-06 e	1.02e-07 a	3.40e-01 a
Bis(2-chloroethyl)ether	111-44-4	5.67E-02 e	8.71E-06 e	1.80e-05 a	1.72e+04 a
Bis(2-chloroisopropyl)ether	39638-32-9	4.01E-02 e	7.40E-06 e	1.34e-04 d	1.31e+03 a
Bromodichloromethane	75-27-4	5.63E-02 e	1.07E-05 e	1.60e-03 a	6.74e+03 a
Bromomethane (methyl bromide)	74-83-9	1.00E-01 e	1.35E-05 e	6.24e-03 a	1.52e+04 a
Butadiene, 1,3-	106-99-0	1.00E-01 e	1.03E-05 e	7.36e-02 a	7.35e+02 a
Carbon tetrachloride	56-23-5	5.71E-02 e	9.78E-06 e	3.04e-02 a	7.93e+02 a
Carbon disulfide	75-15-0	1.06E-01 e	1.30E-05 e	3.03e-02 a	1.19e+03 a
Chlordane	57-74-9	2.15E-02 e	5.45E-06 e	4.86e-05 a	5.60e-02 a
Chloro-1,3-butadiene, 2- (Chloroprene)	126-99-8	8.41E-02 e	1.00E-05 e	1.19e-02 f	1.74e+03 a
Chlorobenzene	108-90-7	7.21E-02 e	9.48E-06 e	3.70e-03 a	4.72e+02 a
Chlorobenzilate	510-15-6	2.18E-02 e	5.48E-06 e	7.24e-08 f	1.11e+01 a
Chlorodibromomethane	124-48-1	3.66E-02 e	1.06E-05 e	7.83e-04 a	2.60e+03 a
Chloroethane (ethyl chloride)	75-00-3	1.04E-01 e	1.16E-05 e	8.82e-03 a	5.68e+03 a
Chloroform	67-66-3	7.70E-02 e	1.09E-05 e	3.67e-03 a	7.92e+03 a
Chloromethane (methyl chloride)	74-87-3	1.24E-01 e	1.36E-05 e	8.82e-03 a	5.33e+03 a
Chlorophenol, 2-	95-57-8	6.61E-02 e	9.48E-06 e	3.91e-04 a	2.20e+04 a
Chloropropene, 3- (allyl chloride)	107-05-1	9.36E-02 e	1.08E-05 e	1.10e-02 a	3.37e+03 a
Chrysene	218-01-9	2.61E-02 e	6.75E-06 e	9.46e-05 a	1.60e-03 a
Cresol, o-	95-48-7	7.59E-02 e	9.86E-06 e	1.20e-06 a	2.60e+04 a
Cresol, m-	108-39-4	7.29E-02 e	9.32E-06 e	8.65e-07 a	2.27e+04 a

(continued)

Table B-1. (continued)

Contaminant	CASRN	D_a (cm^2/s)	D_w (cm^2/s)	HLC ($atm\text{-}m^3/mol$)	Sol (mg/L)
Cresol, p-	106-44-5	7.24E-02 e	9.24E-06 e	7.92e-07 a	2.15e+04 a
Cresols (total)	1319-77-3	7.37E-02 e	9.48E-06 e	9.52e-07 a	2.34e+04 a
Cumene	98-82-8	6.02E-02 e	7.85E-06 e	1.16e+00 a	6.13e+01 a
Cyclohexanol	108-93-0	7.59E-02 e	9.35E-06 e	1.02e-04 f	4.30e+04 f
DDT, p,p'-	50-29-3	1.83E-02 e	4.44E-06 e	8.10e-06 a	2.50e-02 a
Dibenz(a,h)anthracene	53-70-3	2.36E-02 e	6.02E-06 e	1.47e-08 a	2.49e-03 a
Dibromo-3-chloropropane, 1,2-	96-12-8	3.21E-02 e	8.90E-06 e	1.47e-04 a	1.23e+03 a
Dichlorobenzene, 1,2-	95-50-1	5.62E-02 e	8.92E-06 e	1.90e-03 a	1.56e+02 a
Dichlorobenzene, 1,4-	106-46-7	5.50E-02 e	8.68E-06 e	2.40e-03 a	7.38e+01 a
Dichlorobenzidine, 3,3'-	91-94-1	4.75E-02 b	5.50E-06 b	4.00e-09 a	3.11e+00 a
Dichlorodifluoromethane (Freon 12)	75-71-8	7.60E-02 e	1.08E-05 e	3.43e-01 a	2.80e+02 a
Dichloroethane, 1,1-	75-34-3	8.36E-02 e	1.06E-05 e	5.62e-03 a	5.06e+03 a
Dichloroethane, 1,2-	107-06-2	8.54E-02 e	1.09E-05 e	9.79e-04 a	8.52e+03 a
Dichloroethylene, 1,1-	75-35-4	8.63E-02 e	1.10E-05 e	2.61e-02 a	2.25e+03 a
Dichloropropane, 1,2-	78-87-5	7.33E-02 e	9.73E-06 e	2.80e-03 a	2.80e+03 a
Dichloropropene, trans-1,3-	10061-02-6	7.63E-02 e	1.01E-05 e	1.80e-03 i	2.72e+03 a
Dichloropropene, 1,3- (isomer mixture)	542-75-6	7.63E-02 e	1.01E-05 e	1.77e-02 a	2.80e+03 a
Dichloropropene, cis-1,3-	10061-01-5	7.65E-02 e	1.02E-05 e	2.40e-03 i	2.72e+03 a
Dieldrin	60-57-1	2.33E-02 e	6.01E-06 e	1.51e-05 a	1.95e-01 a
Dimethyl formamide, N,N- (DMF)	68-12-2	9.72E-02 e	1.12E-05 e	7.39e-08 i	1.00e+06 f
Dimethylbenz(a)anthracene, 7,12-	57-97-6	4.71E-02 b	5.45E-06 b	3.11e-08 a	2.50e-02 a
Dinitrotoluene, 2,4-	121-14-2	3.75E-02 e	7.90E-06 e	9.26e-08 a	2.70e+02 a
Dioxane, 1,4-	123-91-1	8.74E-02 e	1.05E-05 e	4.80e-06 a	1.00e+06 a
Diphenylhydrazine, 1,2-	122-66-7	0.0343 e	7.25E-06 e	1.53e-06 a	6.80e+01 a
Epichlorohydrin	106-89-8	0.0888 e	1.11E-05 e	3.04e-05 a	6.59e+04 a
Epoxybutane, 1,2-	106-88-7	9.32E-02 e	1.05E-05 e	1.80e-04 f	9.50e+04 f
Ethoxyethanol acetate, 2-	111-15-9	5.70E-02 e	7.98E-06 e	1.80e-06 i	2.29e+05 i
Ethoxyethanol , 2-	110-80-5	8.19E-02 e	9.76E-06 e	1.23e-07 a	1.00e+06 a
Ethylbenzene	100-41-4	6.86E-02 e	8.48E-06 e	7.88e-03 a	1.69e+02 a
Ethylene dibromide (1,2-dibromoethane)	106-93-4	4.31E-02 e	1.05E-05 e	7.43e-04 a	4.18e+03 a
Ethylene glycol	107-21-1	1.17E-01 e	1.36E-05 e	6.00e-08 a	1.00e+06 a
Ethylene thiourea	96-45-7	8.69E-02 b	1.01E-05 b	3.08e-10 a	6.20e+04 a
Ethylene oxide	75-21-8	1.34E-01 e	1.46E-05 e	1.48e-04 f	1.00e+06 g
Formaldehyde	50-00-0	1.67E-01 e	1.74E-05 e	3.36e-07 a	5.50e+05 a
Furfural	98-01-1	8.53E-02 e	1.07E-05 e	4.00e-06 a	1.10e+05 a
HCH, gamma- (Lindane)	58-89-9	2.74E-02 e	7.30E-06 e	1.40e-05 a	6.80e+00 a

(continued)

Table B-1. (continued)

Contaminant	CASRN	D_a (cm^2/s)	D_w (cm^2/s)	HLC ($atm\text{-}m^3/mol$)	Sol (mg/L)
HCH, beta-	319-85-7	0.0277 e	7.40E-06 e	7.43e-07 a	2.40e-01 a
HCH, alpha-	319-84-6	2.75E-02 e	7.35E-06 e	1.06e-05 a	2.00e+00 a
Heptachlor epoxide	1024-57-3	2.19E-02 e	5.58E-06 e	9.50e-06 a	2.00e-01 a
Heptachlor	76-44-8	2.23E-02 e	5.70E-06 e	1.10e-03 a	1.80e-01 a
Hexachloro-1,3-butadiene	87-68-3	2.67E-02 e	7.03E-06 e	8.15e-03 a	3.23e+00 a
Hexachlorobenzene	118-74-1	2.90E-02 e	7.85E-06 e	1.32e-03 a	5.00e-03 a
Hexachlorocyclopentadiene	77-47-4	2.72E-02 e	7.22E-06 e	2.70e-02 a	1.80e+00 a
Hexachlorodibenzo-p-dioxins (HxCDDs)	34465-46-8	4.27E-02 j	4.12E-06 b	1.10e-05 c	4.40e-06 c
Hexachlorodibenzofurans (HxCDFs)	55684-94-1	4.36E-02 j	4.23E-06 b	1.10e-05 c	1.30e-05 c
Hexachloroethane	67-72-1	3.21E-02 e	8.89E-06 e	3.89e-03 a	5.00e+01 a
Hexane, n-	110-54-3	7.28E-02 e	8.12E-06 e	1.43e-02 a	1.24e+01 a
Indeno(1,2,3-cd)pyrene	193-39-5	4.48E-02 b	5.19E-06 b	1.60e-06 a	2.20e-05 a
Isophorone	78-59-1	5.25E-02 e	7.53E-06 e	6.64e-06 a	1.20e+04 a
Mercury	7439-97-6	7.15E-02 e	3.01E-05 e	7.10e-03 k	5.62e-02 h
Methacrylonitrile	126-98-7	9.64E-02 e	1.06E-05 e	2.47e-04 a	2.54e+04 a
Methanol	67-56-1	1.58E-01 e	1.65E-05 e	4.55e-06 a	1.00e+06 a
Methoxyethanol acetate, 2-	110-49-6	6.59E-02 e	8.71E-06 e	3.11e-07 d	1.00e+06 i
Methoxyethanol, 2-	109-86-4	0.0952 e	1.10E-05 e	8.10e-08 f	1.00e+06 g
Methyl methacrylate	80-62-6	7.53E-02 e	9.25E-06 e	3.37e-04 a	1.50e+04 a
Methyl tert-butyl ether (MTBE)	1634-04-4	7.55E-02 e	8.63E-06 e	5.87e-04 f	5.13e+04 f
Methyl isobutyl ketone	108-10-1	6.98E-02 e	8.36E-06 e	1.38e-04 a	1.90e+04 a
Methyl ethyl ketone	78-93-3	9.17E-02 e	1.02E-05 e	5.59e-05 a	2.23e+05 a
Methylcholanthrene, 3-	56-49-5	2.41E-02 e	6.14E-06 e	9.40e-07 a	3.23e-03 a
Methylene chloride (dichloromethane)	75-09-2	9.99E-02 e	1.25E-05 e	2.19e-03 a	1.30e+04 a
N-Nitrosomethylethylamine	10595-95-6	8.41E-02 e	9.99E-06 e	1.40e-06 i	1.97e+04 a
N-Nitrosodimethylamine	62-75-9	9.88E-02 e	1.15E-05 e	1.20e-06 a	1.00e+06 a
N-Nitrosopiperidine	100-75-4	6.99E-02 e	9.18E-06 e	2.80e-07 a	7.65e+04 a
N-Nitrosodiphenylamine	86-30-6	2.84E-02 e	7.19E-06 e	5.00e-06 a	3.51e+01 a
N-Nitrosodiethylamine	55-18-5	7.38E-02 e	9.13E-06 e	3.63e-06 a	9.30e+04 a
N-Nitroso-di-n-butylamine	924-16-3	4.22E-02 e	6.83E-06 e	3.16e-04 a	1.27e+03 a
N-Nitrosopyrrolidine	930-55-2	8.00E-02 e	1.01E-05 e	1.20e-08 a	1.00e+06 a
N-Nitroso-di-n-propylamine	621-64-7	5.64E-02 e	7.76E-06 e	2.25e-06 a	9.89e+03 a
Naphthalene	91-20-3	6.05E-02 e	8.38E-06 e	4.83e-04 a	3.10e+01 a
Nitrobenzene	98-95-3	6.81E-02 e	9.45E-06 e	2.40e-05 a	2.09e+03 a
Nitropropane, 2-	79-46-9	8.47E-02 e	1.02E-05 e	1.23e-04 a	1.70e+04 a

(continued)

Table B-1. (continued)

Contaminant	CASRN	D_a (cm^2/s)	D_w (cm^2/s)	HLC ($atm\text{-}m^3/mol$)	Sol (mg/L)
Pentachlorodibenzo-p-dioxins (PeCDDs)	36088-22-9	4.47E-02 j	4.38E-06 b	2.60e-06 c	1.18e-04 c
Pentachlorodibenzofurans (PeCDFs)	30402-15-4	4.57E-02 j	4.51E-06 b	5.00e-06 c	2.40e-04 c
Pentachlorophenol	87-86-5	2.95E-02 e	8.01E-06 e	2.44e-08 a	1.95e+03 a
Phenol	108-95-2	8.34E-02 e	1.03E-05 e	3.97e-07 a	8.28e+04 a
Phthalic anhydride	85-44-9	5.95E-02 e	9.75E-06 e	1.63e-08 a	6.20e+03 a
Polychlorinated biphenyls (Aroclors)	1336-36-3	2.33E-02 e	5.98E-06 e	2.60e-03 a	7.00e-02 a
Propylene oxide (1,2-epoxypropane)	75-56-9	1.10E-01 e	1.21E-05 e	1.23e-04 f	4.05e+05 f
Pyridine	110-86-1	9.31E-02 e	1.09E-05 e	8.88e-06 a	1.00e+06 a
Styrene	100-42-5	7.13E-02 e	8.81E-06 e	2.75e-03 a	3.10e+02 a
TCDD, 2,3,7,8-	1746-01-6	4.70E-02 j	4.68E-06 b	3.29e-05 c	1.93e-05 c
Tetrachlorodibenzo-p-dioxins (TCDDs)	41903-57-5	4.70E-02 j	4.68E-06 b	1.70e-05 c	3.30e-04 c
Tetrachlorodibenzofurans (TCDFs)	55722-27-5	4.82E-02 j	4.84E-06 b	1.40e-05 c	4.20e-04 c
Tetrachloroethane, 1,1,2,2-	79-34-5	4.89E-02 e	9.29E-06 e	3.45e-04 a	2.97e+03 a
Tetrachloroethane, 1,1,1,2-	630-20-6	4.82E-02 e	9.10E-06 e	2.42e-03 a	1.10e+03 a
Tetrachloroethylene	127-18-4	5.05E-02 e	9.45E-06 e	1.84e-02 a	2.00e+02 a
Toluene	108-88-3	7.80E-02 e	9.23E-06 e	6.64e-03 a	5.26e+02 a
Toluenediamine 2,4-	95-80-7	7.72E-02 b	8.94E-06 b	7.92e-10 a	3.37e+04 a
Toluidine, o-	95-53-4	7.24E-02 e	9.18E-06 e	2.72e-06 a	1.66e+04 a
Toxaphene (chlorinated camphenes)	8001-35-2	2.16E-02 e	5.48E-06 e	6.00e-06 a	7.40e-01 a
Tribromomethane (bromoform)	75-25-2	3.58E-02 e	1.04E-05 e	5.35e-04 a	3.10e+03 a
Trichloro-1,2,2-trifluoro-ethane, 1,1,2-	76-13-1	3.76E-02 e	8.59E-06 e	4.81e-01 a	1.70e+02 a
Trichlorobenzene, 1,2,4-	120-82-1	3.96E-02 e	8.40E-06 e	1.42e-03 a	3.46e+01 a
Trichloroethane, 1,1,2-	79-00-5	6.69E-02 e	1.00E-05 e	9.13e-04 a	4.42e+03 a
Trichloroethane, 1,1,1-	71-55-6	6.48E-02 e	9.60E-06 e	1.72e-02 a	1.33e+03 a
Trichloroethylene (TCE)	79-01-6	6.87E-02 e	1.02E-05 e	1.03e-02 a	1.10e+03 a
Trichlorofluoromethane (Freon 11)	75-69-4	6.55E-02 e	1.01E-05 e	9.70e-02 a	1.10e+03 a
Trichlorophenol, 2,4,6-	88-06-2	3.14E-02 e	8.09E-06 e	7.79e-06 a	8.00e+02 a
Trichloropropane, 1,2,3-	96-18-4	5.75E-02 e	9.24E-06 e	4.09e-04 a	1.75e+03 a
Triethylamine	121-44-8	6.63E-02 e	7.84E-06 e	1.38e-04 f	5.50e+04 f
Vinyl acetate	108-05-4	8.51E-02 e	1.00E-05 e	5.11e-04 a	2.00e+04 a
Vinyl chloride	75-01-4	1.07E-01 e	1.20E-05 e	2.70e-02 a	2.76e+03 a
Xylene, p-	106-42-3	6.84E-02 e	8.45E-06 e	7.66e-03 a	1.85e+02 a
Xylene, o-	95-47-6	6.91E-02 e	8.56E-06 e	5.19e-03 a	1.78e+02 a
Xylene, m-	108-38-3	6.85E-02 e	8.47E-06 e	7.34e-03 a	1.61e+02 a
Xylenes (total)	1330-20-7	6.87E-02 e	8.49E-06 e	6.73e-03 a	1.75e+02 a

(continued)

Table B-1. (continued)

D_a = air diffusivity; D_w = water diffusivity; HLC = Henry's law constant; Sol = aqueous solubility
CASRN = Chemical Abstract Service Registry Number

Data Sources:
a SCDM (U.S. EPA, 1997b).
b Calculated based on U.S. EPA, 1987.
c U.S. EPA, 2000.
d Calculated based on Lyman, Reehl, and Rosenblatt, 1990.
e Calculated based on WATER9 (U.S. EPA, 2001).
f CHEMFATE (SRC, 1999).
g ChemFinder.com (CambridgeSoft Corporation, 2001).
h The Merck Index (Budavari, 1996).
i HSDB (NLM, 2001).
j Calculated based on U.S. EPA, 2000.
k U.S. EPA, 1997a.

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Attachment A-2

Listing of Input Specifications for Each Unit from WATER9

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Attachment A.1 Listing of Input Specifications for Each Unit from WATER9

Non-aerated units
Run 1 (Tank and SI)

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Type of unit is storage tank
1 Description of unit                        12    RUN1 TANK
2 Wastewater temperature   (C)                     24.52
3 Open surface area of tank  (m2)                  0.9
4 Density of liquid in tank (g/cc)                 1
5 tank waste Mwt, water=18                         18
6 tank storage time (days)                         0
7 tank paint factor                                1
8 tank diameter (m)                                1.1
9 tank vapor space height (m)                      0
10 diurnal temp. change (deg.C)                    11
11 tank height (m)                                 2
12 oil in composite wastewater (wt. %)             0

Type of unit is lagoon
1 Description of unit                        13    RUN1 SI
2 Wastewater temperature   (C)                     24.52
3 Length of impoundment (m)                        6
4 Depth of impoundment (m)                         0.1
5 Width of impoundment (m)                         6
6 active biomass, impoundment (g/l)                0
7 if there is plug flow, enter 1                   0
8 time for emissions in lagoon (months)            0
9 Overall biorate (mg/g bio-hr)                    19

Type of unit is solids removal stream
1 Description of unit                        14    RUN1 TANK SOLIDS
2 flow diversion rate (l/s)                        3.66E-06
3 fraction solids in waste diverted                0.63

Type of unit is hard piped, no headspace
1 Description of unit                        16    RUN1 TANK PIPE
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is hard piped, no headspace
1 Description of unit                        17    RUN1 TANK PIPE
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is solids removal stream
1 Description of unit                        18    RUN1 SI SOLIDS
2 flow diversion rate (l/s)                        3.66E-06
3 fraction solids in waste diverted                0.63

Type of unit is hard piped, no headspace
1 Description of unit                        20    RUN1 SI PIPE
```

```
2 Underflow T (C)                                   25
3 Total water added at the unit (l/s)               0
7 Open surface=1                                    0
8 Subsurface entrance=1                             1
9 subsurface exit =1                                1
10 radius of underflow conduit (cm)                 12
11 distance to next unit (cm)                       500
12 slope of underflow conduit                       0.015

Type of unit is hard piped, no headspace
1 Description of unit                          21   RUN1 SI PIPE
2 Underflow T (C)                                   25
3 Total water added at the unit (l/s)               0
7 Open surface=1                                    0
8 Subsurface entrance=1                             1
9 subsurface exit =1                                1
10 radius of underflow conduit (cm)                 12
11 distance to next unit (cm)                       500
12 slope of underflow conduit                       0.015
```

Non-aerated Units
Run 2 (SI only)

```
Type of unit is hard piped, no headspace
1 Description of unit                        24    RUN2 SI PIPE
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is hard piped, no headspace
1 Description of unit                        25    RUN2 SI PIPE
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is lagoon
1 Description of unit                        26    RUN2 SI
2 Wastewater temperature   (C)                     24.52
3 Length of impoundment (m)                        8
4 Depth of impoundment (m)                         0.2
5 Width of impoundment (m)                         8
6 active biomass, impoundment (g/l)                0.03
7 if there is plug flow, enter 1                   0
8 time for emissions in lagoon (months)            0
9 Overall biorate (mg/g bio-hr)                    19

Type of unit is solids removal stream
1 Description of unit                        27    RUN2 SI SOLIDS
2 flow diversion rate (l/s)                        6.39E-06
3 fraction solids in waste diverted                0.63
```

Non-aerated Units
Run 3 (Tank and SI)

```
Type of unit is storage tank
1 Description of unit                          12    RUN3 TANK
2 Wastewater temperature   (C)                       24.52
3 Open surface area of tank  (m2)                    6.6
4 Density of liquid in tank (g/cc)                   1
5 tank waste Mwt, water=18                           18
6 tank storage time (days)                           0
7 tank paint factor                                  1
8 tank diameter (m)                                  2.9
9 tank vapor space height (m)                        0
10 diurnal temp. change (deg.C)                      11
11 tank height (m)                                   2.6
12 oil in composite wastewater (wt. %)               0

Type of unit is lagoon
1 Description of unit                          13    RUN3 SI
2 Wastewater temperature   (C)                       24.52
3 Length of impoundment (m)                          48
4 Depth of impoundment (m)                           0.9
5 Width of impoundment (m)                           48
6 active biomass, impoundment (g/l)                  0
7 if there is plug flow, enter 1                     0
8 time for emissions in lagoon (months)              0
9 Overall biorate (mg/g bio-hr)                      19

Type of unit is solids removal stream
1 Description of unit                          14    RUN3 TANK SOLIDS
2 flow diversion rate (l/s)                          0.00134
3 fraction solids in waste diverted                  0.63

Type of unit is hard piped, no headspace
1 Description of unit                          16    RUN3 TANK PIPE
2 Underflow T (C)                                    25
3 Total water added at the unit (l/s)                0
7 Open surface=1                                     0
8 Subsurface entrance=1                              1
9 subsurface exit =1                                 1
10 radius of underflow conduit (cm)                  12
11 distance to next unit (cm)                        500
12 slope of underflow conduit                        0.015

Type of unit is hard piped, no headspace
1 Description of unit                          17    RUN3 TANK PIPE
2 Underflow T (C)                                    25
3 Total water added at the unit (l/s)                0
7 Open surface=1                                     0
8 Subsurface entrance=1                              1
9 subsurface exit =1                                 1
10 radius of underflow conduit (cm)                  12
11 distance to next unit (cm)                        500
12 slope of underflow conduit                        0.015

Type of unit is solids removal stream
1 Description of unit                          18    RUN3 SI SOLIDS
2 flow diversion rate (l/s)                          0.00134
3 fraction solids in waste diverted                  0.63

Type of unit is hard piped, no headspace
1 Description of unit                          20    RUN3 SI PIPE
2 Underflow T (C)                                    25
3 Total water added at the unit (l/s)                0
7 Open surface=1                                     0
```

```
8 Subsurface entrance=1                          1
9 subsurface exit =1                             1
10 radius of underflow conduit (cm)              12
11 distance to next unit (cm)                    500
12 slope of underflow conduit                    0.015

Type of unit is hard piped, no headspace
1 Description of unit                       21   RUN3 SI PIPE
2 Underflow T (C)                                25
3 Total water added at the unit (l/s)            0
7 Open surface=1                                 0
8 Subsurface entrance=1                          1
9 subsurface exit =1                             1
10 radius of underflow conduit (cm)              12
11 distance to next unit (cm)                    500
12 slope of underflow conduit                    0.015
```

Non-aerated Units
Run 4 (SI only)

```
Type of unit is hard piped, no headspace
1 Description of unit                        24    RUN4 SI PIPE
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is hard piped, no headspace
1 Description of unit                        25    RUN4 SI PIPE
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is lagoon
1 Description of unit                        26    RUN4 SI
2 Wastewater temperature   (C)                     24.52
3 Length of impoundment (m)                        17
4 Depth of impoundment (m)                         0.4
5 Width of impoundment (m)                         17
6 active biomass, impoundment (g/l)                0.03
7 if there is plug flow, enter 1                   0
8 time for emissions in lagoon (months)            0
9 Overall biorate (mg/g bio-hr)                    19

Type of unit is solids removal stream
1 Description of unit                        27    RUN4 SI SOLIDS
2 flow diversion rate (l/s)                        0.00137
3 fraction solids in waste diverted                0.63
```

Type of unit is storage tank		
1 Description of unit	12	RUN5 TANK
2 Wastewater temperature (C)		24.52
3 Open surface area of tank (m2)		6
4 Density of liquid in tank (g/cc)		1
5 tank waste Mwt, water=18		18
6 tank storage time (days)		0
7 tank paint factor		1
8 tank diameter (m)		2.7
9 tank vapor space height (m)		0
10 diurnal temp. change (deg.C)		11
11 tank height (m)		2.5
12 oil in composite wastewater (wt. %)		0
Type of unit is lagoon		
1 Description of unit	13	RUN5 SI
2 Wastewater temperature (C)		24.52
3 Length of impoundment (m)		8
4 Depth of impoundment (m)		0.2
5 Width of impoundment (m)		8
6 active biomass, impoundment (g/l)		0
7 if there is plug flow, enter 1		0
8 time for emissions in lagoon (months)		0
9 Overall biorate (mg/g bio-hr)		19
Type of unit is solids removal stream		
1 Description of unit	14	RUN5 TANK SOLIDS
2 flow diversion rate (l/s)		1.84E-06
3 fraction solids in waste diverted		0.99
Type of unit is hard piped, no headspace		
1 Description of unit	16	RUN5 TANK PIPE
2 Underflow T (C)		25
3 Total water added at the unit (l/s)		0
7 Open surface=1		0
8 Subsurface entrance=1		1
9 subsurface exit =1		1
10 radius of underflow conduit (cm)		12
11 distance to next unit (cm)		500
12 slope of underflow conduit		0.015
Type of unit is hard piped, no headspace		
1 Description of unit	17	RUN5 TANK PIPE
2 Underflow T (C)		25
3 Total water added at the unit (l/s)		0
7 Open surface=1		0
8 Subsurface entrance=1		1
9 subsurface exit =1		1
10 radius of underflow conduit (cm)		12
11 distance to next unit (cm)		500
12 slope of underflow conduit		0.015
Type of unit is solids removal stream		
1 Description of unit	18	RUN5 SI SOLIDS
2 flow diversion rate (l/s)		1.84E-06
3 fraction solids in waste diverted		0.99
Type of unit is hard piped, no headspace		
1 Description of unit	20	RUN5 SI PIPE
2 Underflow T (C)		25
3 Total water added at the unit (l/s)		0
7 Open surface=1		0

```
8 Subsurface entrance=1                          1
9 subsurface exit =1                             1
10 radius of underflow conduit (cm)              12
11 distance to next unit (cm)                    500
12 slope of underflow conduit                    0.015

Type of unit is hard piped, no headspace
1 Description of unit                       21   RUN5 SI PIPE
2 Underflow T (C)                                25
3 Total water added at the unit (l/s)            0
7 Open surface=1                                 0
8 Subsurface entrance=1                          1
9 subsurface exit =1                             1
10 radius of underflow conduit (cm)              12
11 distance to next unit (cm)                    500
12 slope of underflow conduit                    0.015
```

```
Type of unit is hard piped, no headspace
1 Description of unit                        1     inlet pipe
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is hard piped, no headspace
1 Description of unit                        2     transfer pipe
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is primary municipal clarifier
1 Description of unit                        4     Primary clarifier
2 Wastewater temperature   (C)                     25
3 primary clarifier diameter (m)                   1
4 primary clarifier depth  (m)                     2
5 clarifier solids removal efficiency              0.6
6 waterfall drop height (cm)                       20
7 clarifier weir/circumference                     0.5
8 Center well present, =1                          1
10 number of identical units in parallel           0
15 vent air emission control factor                0
16 cover vent rate (m3/s per m2 surface)           0.0005
17 If covered, then enter 1                        0

Type of unit is activated sludge
1 Description of unit                        5     Activated Sludge
2 Wastewater temperature   (C)                     25
3 length of aeration unit (m)                      1
4 width of aeration unit (m)                       1
5 depth of aeration unit (m)                       3.5
6 Area of agitation (each aerator,m2)              1
7 Total number of agitators in the unit            1
8 Power of agitation (each aerator,HP)             0.014
9 Impeller diameter (cm)                           60
10 Impeller rotation (RPM)                         1200
11 Agitator mechanical efficiency                  0.83
12 aerator effectiveness, alpha                    0.83
13 if there is plug flow, enter 1                  0
14 Overall biorate (mg/g bio-hr)                   19
15 Aeration air flow (m3/s)                        0.001
16 activated sludge biomass(g/l)                   2.5
17 If covered, then enter 1                        0
18 agitator pump rate(m3/s each)                   0

Type of unit is circular clarifier
1 Description of unit                        6     Secondary Clarifier
2 Wastewater temperature   (C)                     25
3 secondary clarifier diameter (m)                 1
4 secondary clarifier depth  (m)                   3
5 clarifier solids removal efficiency              0.99
```

```
6 waterfall drop height (cm)                    20
7 clarifier weir/circumference                  0.5

Type of unit is solids removal stream
1 Description of unit                   7       SecClar sludge split
2 flow diversion rate (l/s)                     0.12
3 fraction solids in waste diverted             0.99

Type of unit is hard piped, no headspace
1 Description of unit                   8       SecClar sludge split
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is hard piped, no headspace
1 Description of unit                   9       Sludge recycle
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is divert flow
1 Description of unit                   10      SecClar wasted sludge
2 flow diversion rate (l/s)                     0.007
4 fraction waste flow diverted                  0

Type of unit is hard piped, no headspace
1 Description of unit                   11      SecClar wasted sludge
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is solids removal stream
1 Description of unit                   12      PrimClar sludge
2 flow diversion rate (l/s)                     0.007
3 fraction solids in waste diverted             0.6

Type of unit is hard piped, no headspace
1 Description of unit                   13      PrimClar sludge
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is hard piped, no headspace
1 Description of unit                   40      Act sludge effluent
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
```

7 Open surface=1		0
8 Subsurface entrance=1		1
9 subsurface exit =1		1
10 radius of underflow conduit (cm)		12
11 distance to next unit (cm)		500
12 slope of underflow conduit		0.015

Type of unit is hard piped, no headspace

1 Description of unit	41	SecClar effluent
2 Underflow T (C)		25
3 Total water added at the unit (l/s)		0
7 Open surface=1		0
8 Subsurface entrance=1		1
9 subsurface exit =1		1
10 radius of underflow conduit (cm)		12
11 distance to next unit (cm)		500
12 slope of underflow conduit		0.015

```
Type of unit is hard piped, no headspace
1 Description of unit                        42    inlet pipe
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is hard piped, no headspace
1 Description of unit                        43    transfer pipe
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is primary municipal clarifier
1 Description of unit                        45    primary clarifier
2 Wastewater temperature   (C)                     25
3 primary clarifier diameter (m)                   3
4 primary clarifier depth  (m)                     3.8
5 clarifier solids removal efficiency              0.6
6 waterfall drop height (cm)                       20
7 clarifier weir/circumference                     0.5
8 Center well present, =1                          1
10 number of identical units in parallel           0
15 vent air emission control factor                0
16 cover vent rate (m3/s per m2 surface)           0.0005
17 If covered, then enter 1                        0

Type of unit is activated sludge
1 Description of unit                        46    Activated Sludge
2 Wastewater temperature   (C)                     25
3 length of aeration unit (m)                      5.2
4 width of aeration unit (m)                       3.5
5 depth of aeration unit (m)                       5
6 Area of agitation (each aerator,m2)              47
7 Total number of agitators in the unit            1
8 Power of agitation (each aerator,HP)             0.34
9 Impeller diameter (cm)                           60
10 Impeller rotation (RPM)                         1200
11 Agitator mechanical efficiency                  0.83
12 aerator effectiveness, alpha                    0.83
13 if there is plug flow, enter 1                  0
14 Overall biorate (mg/g bio-hr)                   19
15 Aeration air flow (m3/s)                        0.026
16 activated sludge biomass(g/l)                   2.5
17 If covered, then enter 1                        0
18 agitator pump rate(m3/s each)                   0

Type of unit is circular clarifier
1 Description of unit                        47    Secondary Clarifie
2 Wastewater temperature   (C)                     25
3 secondary clarifier diameter (m)                 4
4 secondary clarifier depth  (m)                   4
5 clarifier solids removal efficiency              0.99
```

```
6 waterfall drop height (cm)                    20
7 clarifier weir/circumference                  0.5

Type of unit is solids removal stream
1 Description of unit                   48      SecClar sludge split
2 flow diversion rate (l/s)                     0.12
3 fraction solids in waste diverted             0.99

Type of unit is hard piped, no headspace
1 Description of unit                   49      SecClar sludge split
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is hard piped, no headspace
1 Total water added at the unit (l/s)   50       SecClar sludge recycle
2 Area of openings at unit (cm2)                 50
3 Radius of drop pipe (cm)                       5
4 Drop length to conduit (cm)                    61
5 Humidity of inlet air (%)                      60
6 Temperature of air (C)                         10.16
7 Drain air velocity (ft/min)                    84
8 manhole air velocity (ft/min)                  128
9 Conduit air velocity (ft/min)                  66
10 Wind velocity (cm/s at 10 m)                  377
11 distance to next unit (cm)                    500
12 slope of underflow conduit                    .015
13 friction factor liquid                        .016
14 friction factor gas                           .006
15 radius of underflow conduit (cm)              12
16 Underflow T (C)                               25
17 oscillation cycle time (min)                  5
18 design collection velocities  (ft/s)          2

Type of unit is divert flow
1 Description of unit                   51      SecClar wasted sludge
8 oil molecular weight                           180
9 oil density  (g/cc)                            .8
10 NaUT 1=municipal 2=industrial                 0
11 NaUT 1=mass tr. 2=equil                       0

Type of unit is hard piped, no headspace
1 Description of unit                   52      SecClar wasted sludge
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is solids removal stream
1 Description of unit                   53      PrimClar sludge
2 flow diversion rate (l/s)                     0.007
3 fraction solids in waste diverted             0.6

Type of unit is hard piped, no headspace
1 Description of unit                   54      PrimClar sludge
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
```

7 Open surface=1		0
8 Subsurface entrance=1		1
9 subsurface exit =1		1
10 radius of underflow conduit (cm)		12
11 distance to next unit (cm)		500
12 slope of underflow conduit		0.015

Type of unit is hard piped, no headspace

1 Description of unit	81	Act sludge effluent
2 Underflow T (C)		25
3 Total water added at the unit (l/s)		0
7 Open surface=1		0
8 Subsurface entrance=1		1
9 subsurface exit =1		1
10 radius of underflow conduit (cm)		12
11 distance to next unit (cm)		500
12 slope of underflow conduit		0.015

Type of unit is hard piped, no headspace

1 Description of unit	82	SecClar effluent
2 Underflow T (C)		25
3 Total water added at the unit (l/s)		0
7 Open surface=1		0
8 Subsurface entrance=1		1
9 subsurface exit =1		1
10 radius of underflow conduit (cm)		12
11 distance to next unit (cm)		500
12 slope of underflow conduit		0.015

```
Type of unit is hard piped, no headspace
1 Description of unit                        1     inlet pipe
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is hard piped, no headspace
1 Description of unit                        2     transfer pip
2 Underflow T (C)                                  25
3 Total water added at the unit (l/s)              0
7 Open surface=1                                   0
8 Subsurface entrance=1                            1
9 subsurface exit =1                               1
10 radius of underflow conduit (cm)                12
11 distance to next unit (cm)                      500
12 slope of underflow conduit                      0.015

Type of unit is primary municipal clarifier
1 Description of unit                        4     primary clarifier
2 Wastewater temperature   (C)                     25
3 primary clarifier diameter (m)                   1
4 primary clarifier depth  (m)                     2
5 clarifier solids removal efficiency              0.6
6 waterfall drop height (cm)                       20
7 clarifier weir/circumference                     0.5
8 Center well present, =1                          1
10 number of identical units in parallel           0
15 vent air emission control factor                0
16 cover vent rate (m3/s per m2 surface)           0.0005
17 If covered, then enter 1                        0

Type of unit is activated sludge
1 Description of unit                        5     Activated Sludge
2 Wastewater temperature   (C)                     25
3 length of aeration unit (m)                      0.8
4 width of aeration unit (m)                       0.8
5 depth of aeration unit (m)                       2.5
6 Area of agitation (each aerator,m2)              1
7 Total number of agitators in the unit            1
8 Power of agitation (each aerator,HP)             0.006
9 Impeller diameter (cm)                           60
10 Impeller rotation (RPM)                         1200
11 Agitator mechanical efficiency                  0.83
12 aerator effectiveness, alpha                    0.83
13 if there is plug flow, enter 1                  0
14 Overall biorate (mg/g bio-hr)                   19
15 Aeration air flow (m3/s)                        0.00044
16 activated sludge biomass(g/l)                   2.5
17 If covered, then enter 1                        0
18 agitator pump rate(m3/s each)                   0

Type of unit is circular clarifier
1 Description of unit                        6     Secondary Clarifier
2 Wastewater temperature   (C)                     25
3 secondary clarifier diameter (m)                 1
4 secondary clarifier depth  (m)                   3
5 clarifier solids removal efficiency              0.99
```

```
6 waterfall drop height (cm)                    20
7 clarifier weir/circumference                  0.5

Type of unit is solids removal stream
1 Description of unit                   7       SecClar sludge split
2 flow diversion rate (l/s)                     0.12
3 fraction solids in waste diverted             0.99

Type of unit is hard piped, no headspace
1 Description of unit                   8       SecClar sludge split
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is hard piped, no headspace
1 Description of unit                   9       SecClar Sludge recycle
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is divert flow
1 Description of unit                   10      SecClar wasted sludge
2 flow diversion rate (l/s)                     0.007
4 fraction waste flow diverted                  0

Type of unit is hard piped, no headspace
1 Description of unit                   11      SecClar wasted sludge
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is solids removal stream
1 Description of unit                   12      PrimClar sludge
2 flow diversion rate (l/s)                     0.007
3 fraction solids in waste diverted             0.6

Type of unit is hard piped, no headspace
1 Description of unit                   13      PrimClar sludge
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
7 Open surface=1                                0
8 Subsurface entrance=1                         1
9 subsurface exit =1                            1
10 radius of underflow conduit (cm)             12
11 distance to next unit (cm)                   500
12 slope of underflow conduit                   0.015

Type of unit is hard piped, no headspace
1 Description of unit                   40      Act sludge effluent
2 Underflow T (C)                               25
3 Total water added at the unit (l/s)           0
```

7 Open surface=1		0
8 Subsurface entrance=1		1
9 subsurface exit =1		1
10 radius of underflow conduit (cm)		12
11 distance to next unit (cm)		500
12 slope of underflow conduit		0.015

Type of unit is hard piped, no headspace

1 Description of unit	41	SecClar effluent
2 Underflow T (C)		25
3 Total water added at the unit (l/s)		0
7 Open surface=1		0
8 Subsurface entrance=1		1
9 subsurface exit =1		1
10 radius of underflow conduit (cm)		12
11 distance to next unit (cm)		500
12 slope of underflow conduit		0.015

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Attachment A-3

Toxicity Benchmarks Used in the Industrial Waste Evaluation Model (IWEM)

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MEMORANDUM

DATE: August 27, 2001

TO: Ann Johnson

FROM: Susan N. Wolf, Robert S. Truesdale

SUBJECT: Toxicity benchmarks used in the Industrial Waste Evaluation Model (IWEM) *(revised)*

Human health benchmarks for chronic oral and inhalation exposures were used in the Industrial Waste Evaluation Model (IWEM). The U.S. Environmental Protection Agency (EPA) uses reference doses (RfDs) and reference concentrations (RfCs) to evaluate noncancer risk from oral and inhalation exposures, respectively. Oral cancer slope factors (CSFs), inhalation unit risk factors (URFs), and inhalation CSFs are used to evaluate risk for carcinogens.

This memorandum provides the toxicity benchmarks used in IWEM. Section 1.0 describes the data sources and general hierarchy used to collect these benchmarks. Section 2.0 provides the benchmarks along with discussions of individual human health benchmarks extracted from a variety of sources.

1.0 Methodology and Data Sources

Several sources of health benchmarks are available. Human health benchmarks were obtained from these sources in the following order of preference:

- Integrated Risk Information System (IRIS)
- Superfund Technical Support Center Provisional Benchmarks
- Health Effects Assessment Summary Tables (HEAST)
- Agency for Toxic Substances and Disease Registry (ATSDR) minimal risk levels (MRLs)
- California Environmental Protection Agency (CalEPA) chronic inhalation reference exposure levels (RELs) and cancer potency factors.
- EPA health assessment documents
- Various other EPA health benchmark sources.

For dioxins and dibenzofurans, World Health Organization (WHO) toxicity equivalency factors (TEFs) from Van den Berg et al. (1998) were applied to the HEAST CSF for 2,3,7,8-TCDD to get CSFs for all other dioxins and furans (see Section 2.4).

- **Integrated Risk Information System (IRIS)**

Benchmarks in IRIS are prepared and maintained by EPA, and values from IRIS were used in IWEM whenever available. IRIS is EPA's electronic database containing information on human health effects (U.S. EPA, 2001a). Each chemical file contains descriptive and quantitative information on potential health effects. Health benchmarks for chronic noncarcinogenic health effects include RfDs and RfCs. Cancer classification, oral CSFs, and inhalation URFs are included for carcinogenic effects. IRIS is the official repository of Agency-wide consensus of human health risk information.

Inhalation CSFs are not available from IRIS, so they were calculated from inhalation URFs (which are available from IRIS) using the following equation:

$$\text{inh CSF} = \text{inh URF} \times 70\ \text{kg} \div 20\ \text{m}^3/\text{d} \times 1000\ \mu\text{g/mg}$$

In this equation, 70 kg represents average body weight; 20 m3/d represents average inhalation rate; and 1000 μg/mg is a units conversion factor (U.S. EPA, 1997). These standard estimates of body weight and inhalation rate are used by EPA in the calculation of the URF, and, therefore, the values were used to calculate inhalation CSFs.

1.2 Superfund Provisional Benchmarks

The Superfund Technical Support Center (EPA's National Center for Environmental Assessment [NCEA]) derives provisional RfCs, RfDs, and CSFs for certain chemicals. These provisional health benchmarks can be found in Risk Assessment Issue Papers. Some of the provisional values have been externally peer reviewed, and some (e.g., trichloroethylene, tetrachloroethylene) come from previously published EPA Health Assessment Documents. These provisional values have not undergone EPA's formal review process for finalizing benchmarks and do not represent Agency-wide consensus information. Specific provisional values used in IWEM are described in Section 2.5.

1.3 Health Effects Summary Tables (HEAST)

HEAST is a listing of provisional noncarcinogenic and carcinogenic health toxicity values (RfDs, RfCs, URFs, and CSFs) derived by EPA (U.S. EPA, 1997). Although the health toxicity values in HEAST have undergone review and have the concurrence of individual EPA program offices, either they have not been reviewed as extensively as those in IRIS or their data set is not complete enough to be listed in IRIS. HEAST benchmarks have not been updated in several years and do not represent Agency-wide consensus information.

1.4 ATSDR Minimal Risk Levels

The ATSDR MRLs are substance-specific health guidance levels for noncarcinogenic endpoints (ATSDR, 2001). An MRL is an estimate of the daily human exposure to a hazardous substance that is likely to be without appreciable risk of adverse noncancer health effects over a specified duration of exposure. MRLs are based on noncancer health effects only and are not based on a consideration of cancer effects. MRLs are derived for acute, intermediate, and chronic exposure durations for oral and inhalation routes of exposure. Inhalation and oral MRLs are derived in a manner similar to EPA's RfCs and RfDs, respectively (i.e., ATSDR uses the no-observed-adverse-effect-level/uncertainty factor (NOAEL/UF) approach); however, MRLs are intended to serve as screening levels and are exposure duration-specific. Also, ATSDR uses EPA's 1994 inhalation dosimetry methodology in the derivation of inhalation MRLs. A chronic inhalation MRL for mixed xylenes was used as a surrogate for each of the xylene isomers.

1.5 CalEPA Cancer Potency Factors and Reference Exposure Levels

CalEPA has developed cancer potency factors for chemicals regulated under California's Hot Spots Air Toxics Program (CalEPA, 1999a). The cancer potency factors are analogous to EPA's oral and inhalation CSFs. CalEPA has also developed chronic inhalation RELs, analogous to EPA's RfC, for 120 substances (CalEPA, 1999b, 2000). CalEPA used EPA's 1994 inhalation dosimetry methodology in the derivation of inhalation RELs. The cancer potency factors and inhalation RELs have undergone internal peer review by various California agencies and have been the subject of public comment. A chronic inhalation REL for mixed cresols was used as a surrogate for each of the cresol isomers.

1.6 Other EPA Health Benchmarks

EPA has also derived health benchmark values in other risk assessment documents, such as Health Assessment Documents (HADs), Health Effect Assessments (HEAs), Health and Environmental Effects Profiles (HEEPs), Health and Environmental Effects Documents (HEEDs), Drinking Water Criteria Documents, and Ambient Water Quality Criteria Documents. Evaluations of potential carcinogenicity of chemicals in support of reportable quantity adjustments were published by EPA's Carcinogen Assessment Group (CAG) and may include cancer potency factor estimates. Health toxicity values identified in these EPA documents are usually dated and are not recognized as Agency-wide consensus information or verified benchmarks, however, and as a result they are used in the hierarchy only when values are not available from IRIS, HEAST, Superfund provisional values, ATSDR, or CalEPA. Section 2.6 describes the specific values from these alternative EPA sources that were used in IWEM.

2.0 IWEM Human Health Benchmarks

The chronic human health benchmarks used to calculate the health-based numbers (HBNs) in IWEM are summarized in Table 1, which provides the Chemical Abstract Service Registry Number (CASRN), constituent name, RfD (mg/kg-d), RfC (mg/m^3), oral CSF

(mg/kg-d^{-1}), inhalation URF [$(\mu g/m^3)^{-1}$], inhalation CSF (mg/kg-d^{-1}), and reference for each benchmark. A key to the references cited and abbreviations used is provided at the end of the table.

For a majority of IWEM constituents, human health benchmarks were available from IRIS (U.S. EPA, 2001a), Superfund Provisional Benchmarks, or HEAST (U.S. EPA, 1997). Benchmarks also were obtained from ATSDR (2001) or CalEPA (1999a, 1999b, 2000). This section describes benchmarks obtained from other sources, along with the Superfund Provisional values and special uses (e.g., benzene, vinyl chloride) of IRIS benchmarks.

2.1 Benzene

The cancer risk estimates for benzene are provided as ranges in IRIS. The oral CSF for benzene is 1.5E-02 to 5.5E-02 $(mg/kg/d)^{-1}$ and the inhalation URF is 2.2E-06 to 7.8E-06 $(\mu g/m^3)^{-1}$ (U.S. EPA, 2001a). For IWEM, the upper range estimates were used (i.e., 5.5E-02 $(mg/kg/d)^{-1}$ and 7.8E-06 $(\mu g/m^3)^{-1}$ for the oral CSF and inhalation URF, respectively).

2.2 Vinyl Chloride

Based on use of the linearized multistage model, IRIS recommends an oral CSF of 7.2E-1 per mg/kg-d for vinyl chloride to account for continuous lifetime exposure during adulthood; this value was used for IWEM.[1] Based on use of the linearized multistage model, an inhalation URF of 4.4E-6 per $\mu g/m^3$ to account for continuous, lifetime exposure during adulthood was recommended for vinyl chloride and was used for IWEM; an inhalation CSF of 1.5E-2 per mg/kg-d was calculated from the URF.[2]

2.3 Polychlorinated Biphenyls

There are two inhalation CSFs available from IRIS for polychlorinated biphenyls (PCBs): 0.4 per mg/kg-d for evaporated congeners and 2.0 per mg/kg-d for dust or aerosol (high risk and persistence). The inhalation CSF for evaporated congeners will be used for IWEM.

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[1]A twofold increase of the oral CSF to 1.4 per mg/kg-d to account for continuous lifetime exposure from birth was also recommended but was not used for IWEM.

[2]A twofold increase to 8.8E-6 per $\mu g/m^3$ for the inhalation URF, to account for continuous lifetime exposure from birth, was also recommended but was not used for IWEM.

Table 1. Human Health Benchmarks Used in IWEM

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Acenaphthene	83-32-9	6.0E-02	I								
Acetaldehyde (ethanal)	75-07-0					9.0E-03	I	2.2E-06	I	7.7E-03	calc
Acetone (2-propanone)	67-64-1	1.0E-01	I			3.1E+01	A				
Acetonitrile (methyl cyanide)	75-05-8					6.0E-02	I				
Acetophenone	98-86-2	1.0E-01	I								
Acrolein	107-02-8	2.0E-02	H			2.0E-05	I				
Acrylamide	79-06-1	2.0E-04	I	4.5E+0	I			1.3E-03	I	4.6E+00	calc
Acrylic acid (propenoic acid)	79-10-7	5.0E-01	I			1.0E-03	I				
Acrylonitrile	107-13-1	1.0E-03	H	5.4E-1	I	2.0E-03	I	6.8E-05	I	2.4E-01	calc
Aldrin	309-00-2	3.0E-05	I	1.7E+01	I			4.9E-03	I	1.7E+01	calc
Allyl alcohol	107-18-6	5.0E-03	I								
Aniline (benzeneamine)	62-53-3			5.7E-3	I	1.0E-03	I	1.6E-06	C99a	5.6E-03	calc
Anthracene	120-12-7	3.0E-01	I								
Antimony	7440-36-0	4.0E-04	I								
Arsenic	7440-38-2	3.0E-04	I	1.5E+00	I						
Barium	7440-39-3	7.0E-02	I								
Benz{a}anthracene	56-55-3			1.2E+00	C99a			1.1E-04	C99a	3.9E-01	calc
Benzene	71-43-2			5.5E-02	I	6.0E-02	C00	7.8E-06	I	2.7E-02	calc
Benzidine	92-87-5	3.0E-03	I	2.3E+02	I			6.7E-02	I	2.3E+02	I
Benzo{a}pyrene	50-32-8			7.3E+00	I			1.1E-03	C99a	3.9E+00	calc
Benzo{b}fluoranthene	205-99-2			1.2E+00	C99a			1.1E-04	C99a	3.9E-01	calc
Benzyl chloride	100-44-7			1.7E-01	I			4.9E-05	C99a	1.7E-01	calc
Benzyl alcohol	100-51-6	3.0E-01	H								

Table 1. Human Health Benchmarks Used in IWEM (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Beryllium	7440-41-7	2.0E-03	I								
Bis(2-chloroethyl)ether	111-44-4			1.1E+00	I			3.3E-04	I	1.2E+00	calc
Bis(2-chloroisopropyl)ether	39638-32-9	4.0E-02	I	7.0E-02	H			1.0E-05	H	3.5E-02	calc
Bis(2-ethylhexyl)phthalate	117-81-7	2.0E-02	I	1.4E-02	I	1.0E-02	C99b	2.4E-06	C99a	8.4E-03	calc
Bromodichloromethane	75-27-4	2.0E-02	I	6.2E-2	I			1.8E-05	AC	6.2E-02	AC
Bromomethane (methyl bromide)	74-83-9	1.4E-03	I			5.0E-03	I				
Butadiene, 1,3-	106-99-0					2.0E-02	C00	2.8E-04	I	9.8E-01	calc
Butanol	71-36-3	1.0E-01	I								
Butyl benzyl phthalate	85-68-7	2.0E-01	I								
Butyl-4,6-dinitrophenol,2-sec- (Dinoseb)	88-85-7	1.0E-03	I								
Cadmium	7440-43-9	5.0E-04	I								
Carbon tetrachloride	56-23-5	7.0E-04	I	1.3E-1	I	7.0E-03	SF	1.5E-05	I	5.3E-02	calc
Carbon disulfide	75-15-0	1.0E-01	I			7.0E-01	I				
Chlordane	57-74-9	5.0E-04	I	3.5E-01	I	7.0E-04	I	1.0E-04	I	3.5E-01	calc
Chloro-1,3-butadiene, 2- (Chloroprene)	126-99-8	2.0E-02	H			7.0E-03	H				
Chloroaniline, p-	106-47-8	4.0E-03	I								
Chlorobenzene	108-90-7	2.0E-02	I			6.0E-02	SF				
Chlorobenzilate	510-15-6	2.0E-02	I	2.7E-01	H			7.8E-05	H	2.7E-01	calc
Chlorodibromomethane	124-48-1	2.0E-02	I	8.4E-2	I			2.4E-05	AC	8.4E-02	AC
Chloroethane (ethyl chloride)	75-00-3					1.0E+01	I				
Chloroform	67-66-3	1.0E-02	I			1.0E-01	A				
Chloromethane (methyl chloride)	74-87-3			1.3E-2	H	9.0E-02	I	1.8E-06	H	6.3E-03	calc
Chlorophenol, 2-	95-57-8	5.0E-03	I			1.4E-03	AC				
Chloropropene, 3- (allyl chloride)	107-05-1					1.0E-03	I	6.0E-06	C99a	2.1E-02	calc
Chromium (III)	16065-83-1	1.5E+00	I								
Chromium (VI)	18540-29-9	3.0E-03	I								
Chrysene	218-01-9			1.2E-01	C99a			1.1E-05	C99a	3.9E-02	calc

Table 1. Human Health Benchmarks Used in IWEM (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Cobalt	7440-48-4	2.0E-02	SF								
Copper	7440-50-8	*MCL only									
Cresol, p-	106-44-5	5.0E-03	H			6.0E-01	surr (C00)				
Cresol, o-	95-48-7	5.0E-02	I			6.0E-01	surr (C00)				
Cresol, m-	108-39-4	5.0E-02	I			6.0E-01	surr (C00)				
Cresols (total)	1319-77-3	5.0E-02	surr (I)			6.0E-01	C00				
Cumene	98-82-8	1.0E-01	I			4.0E-01	I				
Cyclohexanol	108-93-0	1.7E-05	solv			2.0E-05	solv				
Cyclohexanone	108-94-1	5.0E+00	I								
DDD	72-54-8			2.4E-01	I						
DDE	72-55-9			3.4E-01	I						
DDT, p,p'-	50-29-3	5.0E-04	I	3.4E-01	I			9.7E-05	I	3.4E-01	calc
Di-n-butyl phthalate	84-74-2	1.0E-01	I								
Di-n-octyl phthalate	117-84-0	2.0E-02	H								
Diallate	2303-16-4			6.1E-02	H						
Dibenz{a,h}anthracene	53-70-3			7.3E+00	TEF			1.2E-03	C99a	4.2E+00	calc
Dibromo-3-chloropropane, 1,2-	96-12-8			1.4E+0	H	2.0E-04	I	6.9E-07	H	2.4E-03	calc
Dichlorobenzene, 1,2-	95-50-1	9.0E-02	I			2.0E-01	H				
Dichlorobenzene, 1,4-	106-46-7			2.4E-2	H	8.0E-01	I	1.1E-05	C99a	3.9E-02	calc
Dichlorobenzidine, 3,3'-	91-94-1			4.5E-01	I			3.4E-04	C99a	1.2E+00	calc
Dichlorodifluoromethane (Freon 12)	75-71-8	2.0E-01	I			2.0E-01	H				
Dichloroethane, 1,2-	107-06-2			9.1E-2	I	2.4E+00	A	2.6E-05	I	9.1E-02	calc
Dichloroethane, 1,1-	75-34-3	1.0E-01	H			5.0E-01	H	1.6E-06	C99a	5.6E-03	calc
Dichloroethylene, 1,1-	75-35-4	9.0E-03	I	6.0E-1	I	7.0E-02	C00	5.0E-05	I	1.8E-01	calc
Dichloroethylene, *trans*-1,2-	156-60-5	2.0E-02	I								
Dichloroethylene, cis-1,2-	156-59-2	1.0E-02	H								
Dichlorophenol, 2,4-	120-83-2	3.0E-03	I								

Table 1. Human Health Benchmarks Used in IWEM (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Dichlorophenoxyacetic acid, 2,4- (2,4-D)	94-75-7	1.0E-02	I								
Dichloropropane, 1,2-	78-87-5	9.0E-02	A	6.8E-2	H	4.0E-03	I				
Dichloropropene, *trans*-1,3-	10061-02-6	3.0E-02	I	1.0E-1	I	2.0E-02	surr (I)	4.0E-06	surr (I)	1.4E-02	calc
Dichloropropene, *cis*-1,3-	10061-01-5	3.0E-02	I	1.0E-1	I	2.0E-02	surr (I)	4.0E-06	surr (I)	1.4E-02	calc
Dichloropropene, 1,3- (mixture of isomers)	542-75-6	3.0E-02	I	1.0E-01	I	2.0E-02	I	4.0E-06	I	1.4E-02	calc
Dieldrin	60-57-1	5.0E-05	I	1.6E+01	I			4.6E-03	I	1.6E+01	calc
Diethyl phthalate	84-66-2	8.0E-01	I								
Diethylstilbestrol	56-53-1			4.7E+03	H						
Dimethoate	60-51-5	2.0E-04	I								
Dimethoxybenzidine, 3,3'-	119-90-4			1.4E-02	H						
Dimethyl phthalate	131-11-3										
Dimethyl formamide, N,N- (DMF)	68-12-2	1.0E-01	H			3.0E-02	I				
Dimethylbenz{a}anthracene, 7,12-	57-97-6							7.1E-02	C99a	2.5E+02	calc
Dimethylbenzidine, 3,3'-	119-93-7			9.2E+00	H						
Dimethylphenol, 2,4-	105-67-9	2.0E-02	I								
Dimethylphenol, 3,4-	95-65-8	1.0E-03	I								
Dinitrobenzene, 1,3-	99-65-0	1.0E-04	I								
Dinitrophenol, 2,4-	51-28-5	2.0E-03	I								
Dinitrotoluene, 2,6-	606-20-2	1.0E-03	H	6.8E-01	surr (I)						
Dinitrotoluene, 2,4-	121-14-2	2.0E-03	I	6.8E-01	surr (I)			8.9E-05	C99a	3.1E-01	calc
Dioxane, 1,4-	123-91-1			1.1E-2	I	3.0E+00	C00	7.7E-06	C99a	2.7E-02	calc
Diphenylamine	122-39-4	2.5E-02	I								
Diphenylhydrazine, 1,2-	122-66-7			8.0E-1	I			2.2E-04	I	7.7E-01	calc
Disulfoton	298-04-4	4.0E-05	I								
Endosulfan (Endosulfan I and II,mixture)	115-29-7	6.0E-03	I								
Endrin	72-20-8	3.0E-04	I								
Epichlorohydrin	106-89-8	2.0E-03	H	9.9E-3	I	1.0E-03	I	1.2E-06	I	4.2E-03	calc

Table 1. Human Health Benchmarks Used in IWEM (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Epoxybutane, 1,2-	106-88-7					2.0E-02	I				
Ethoxyethanol acetate, 2-	111-15-9	3.0E-01	H			3.0E-01	C00				
Ethoxyethanol, 2-	110-80-5	4.0E-01	H			2.0E-01	I				
Ethyl acetate	141-78-6	9.0E-01	I								
Ethyl ether	60-29-7	2.0E-01	I								
Ethyl methacrylate	97-63-2	9.0E-02	H								
Ethyl methanesulfonate	62-50-0			2.9E+02	RQ						
Ethylbenzene	100-41-4	1.0E-01	I			1.0E+00	I	1.1E-06	SF	3.9E-03	calc
Ethylene oxide	75-21-8			1.0E+0	H	3.0E-02	C00	1.0E-04	H	3.5E-01	calc
Ethylene dibromide (1,2-dibromoethane)	106-93-4			8.5E+1	I	2.0E-04	H	2.2E-04	I	7.7E-01	calc
Ethylene glycol	107-21-1	2.0E+00	I			4.0E-01	C00				
Ethylene thiourea	96-45-7	8.0E-05	I	1.1E-01	H			1.3E-05	C99a	4.6E-02	calc
Fluoranthene	206-44-0	4.0E-02	I								
Fluorene	86-73-7	4.0E-02	I								
Fluoride	16984-48-8	6.0E-02	surr (I)								
Formaldehyde	50-00-0	2.0E-01	I			9.8E-03	A	1.3E-05	I	4.6E-02	calc
Formic acid	64-18-6	2.0E+00	H								
Furan	110-00-9	1.0E-03	I								
Furfural	98-01-1	3.0E-03	I			5.0E-02	H				
HCH, beta-	319-85-7			1.8E+00	I			5.3E-04	I	1.9E+00	calc
HCH, gamma- (Lindane)	58-89-9	3.0E-04	I	1.3E+00	H			3.1E-04	C99a	1.1E+00	calc
HCH, alpha-	319-84-6	8.0E-03	A	6.3E+00	I			1.8E-03	I	6.3E+00	calc
Heptachlor	76-44-8	5.0E-04	I	4.5E+00	I			1.3E-03	I	4.6E+00	calc
Heptachlor epoxide	1024-57-3	1.3E-05	I	9.1E+00	I			2.6E-03	I	9.1E+00	calc
Hexachloro-1,3-butadiene	87-68-3	3.0E-04	SF	7.8E-2	I			2.2E-05	I	7.7E-02	calc
Hexachlorobenzene	118-74-1	8.0E-04	I	1.6E+0	I			4.6E-04	I	1.6E+00	calc
Hexachlorocyclopentadiene	77-47-4	6.0E-03	I			2.0E-04	I				

Table 1. Human Health Benchmarks Used in IWEM (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Hexachlorodibenzo-p-dioxins (HxCDDs)	34465-46-8			1.5E+04	WHO98			3.3E+00	WHO98	1.5E+04	WHO98
Hexachlorodibenzofurans (HxCDFs)	55684-94-1			1.5E+04	WHO98			3.3E+00	WHO98	1.5E+04	WHO98
Hexachloroethane	67-72-1	1.0E-03	I	1.4E-2	I			4.0E-06	I	1.4E-02	calc
Hexachlorophene	70-30-4	3.0E-04	I								
Hexane, n-	110-54-3	1.1E+01	SF			2.0E-01	I				
Indeno{1,2,3-cd}pyrene	193-39-5			1.2E+00	C99a			1.1E-04	C99a	3.9E-01	calc
Isobutyl alcohol	78-83-1	3.0E-01	I								
Isophorone	78-59-1	2.0E-01	I	9.5E-4	I	2.0E+00	C99b				
Kepone	143-50-0	5.0E-04	A								
Lead	7439-92-1	*MCL only									
Manganese	7439-96-5	4.7E-02	I								
Mercury	7439-97-6	1.0E-04	surr (I)			3.0E-04	I				
Methacrylonitrile	126-98-7	1.0E-04	I			7.0E-04	H				
Methanol	67-56-1	5.0E-01	I			4.0E+00	C00				
Methoxychlor	72-43-5	5.0E-03	I								
Methoxyethanol, 2-	109-86-4	1.0E-03	H			2.0E-02	I				
Methoxyethanol acetate, 2-	110-49-6	2.0E-03	H			9.0E-02	C00				
Methyl parathion	298-00-0	2.5E-04	I								
Methyl methacrylate	80-62-6	1.4E+00	I			7.0E-01	I				
Methyl isobutyl ketone	108-10-1	8.0E-02	H			8.0E-02	H				
Methyl ethyl ketone	78-93-3	6.0E-01	I			1.0E+00	I				
Methyl tert-butyl ether (MTBE)	1634-04-4					3.0E+00	I				
Methylcholanthrene, 3-	56-49-5							6.3E-03	C99a	2.2E+01	calc
Methylene bromide (dibromomethane)	74-95-3	1.0E-02	H								
Methylene Chloride (dichloromethane)	75-09-2	6.0E-02	I	7.5E-3	I	3.0E+00	H	4.7E-07	I	1.6E-03	calc
Molybdenum	7439-98-7	5.0E-03	I								
N-Nitroso-di-n-butylamine	924-16-3			5.4E+0	I			1.6E-03	I	5.6E+00	calc

Table 1. Human Health Benchmarks Used in IWEM (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
N-Nitroso-di-n-propylamine	621-64-7			7.0E+00	I			2.0E-03	C99a	7.0E+00	calc
N-Nitrosodiethylamine	55-18-5			1.5E+2	I			4.3E-02	I	1.5E+02	calc
N-Nitrosodimethylamine	62-75-9	8.00E-06	SF	5.1E+01	I			1.4E-02	I	4.9E+01	calc
N-Nitrosodiphenylamine	86-30-6	2.00E-02	SF	4.9E-03	I			2.6E-06	C99a	9.1E-03	calc
N-Nitrosomethylethylamine	10595-95-6			2.2E+01	I			6.3E-03	C99a	3.7E+00	C99a
N-Nitrosopiperidine	100-75-4							2.7E-03	C99a	9.5E+00	calc
N-Nitrosopyrrolidine	930-55-2			2.1E+0	I			6.1E-04	I	2.1E+00	calc
Naphthalene	91-20-3	2.0E-02	I			3.0E-03	I				
Nickel	7440-02-0	2.0E-02	I								
Nitrobenzene	98-95-3	5.0E-04	I			2.0E-03	H				
Nitropropane, 2-	79-46-9					2.0E-02	I	2.7E-03	H	9.5E+00	calc
Octamethyl pyrophosphoramide	152-16-9	2.0E-03	H								
Parathion (ethyl)	56-38-2	6.0E-03	H								
Pentachlorobenzene	608-93-5	8.0E-04	I								
Pentachlorodibenzo-p-dioxins (PeCDDs)	36088-22-9			1.5E+05	WHO98			3.3E+01	WHO98	1.5E+05	WHO98
Pentachlorodibenzofurans (PeCDFs)	30402-15-4			7.5E+04	WHO98			1.7E+01	WHO98	7.5E+04	WHO98
Pentachloronitrobenzene (PCNB)	82-68-8	3.0E-03	I	2.6E-01	H						
Pentachlorophenol	87-86-5	3.0E-02	I	1.2E-01	I			5.1E-06	C99a	1.8E-02	calc
Phenol	108-95-2	6.0E-01	I			2.0E-01	C00				
Phenyl mercuric acetate	62-38-4	8.0E-05	I								
Phenylenediamine, 1,3-	108-45-2	6.0E-03	I								
Phorate	298-02-2	2.0E-04	H								
Phthalic anhydride	85-44-9	2.0E+00	I			1.2E-01	H				
Polychlorinated biphenyls (Aroclors)	1336-36-3	2.0E-05	surr (I)	4.0E-01	I			1.0E-04	I	4.0E-01	I
Pronamide	23950-58-5	7.5E-02	I								
Propylene oxide (1,2-epoxypropane)	75-56-9			2.4E-1	I	3.0E-02	I	3.7E-06	I	1.3E-02	calc
Pyrene	129-00-0	3.0E-02	I								

Table 1. Human Health Benchmarks Used in IWEM (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Pyridine	110-86-1	1.0E-03	I			7.0E-03	EPA86				
Safrole	94-59-7			1.8E-01	RQ						
Selenium	7782-49-2	5.0E-03	I								
Silver	7440-22-4	5.0E-03	I								
Strychnine and salts	57-24-9	3.0E-04	I								
Styrene	100-42-5	2.0E-01	I			1.0E+00	I				
Tetrachlorobenzene, 1,2,4,5-	95-94-3	3.0E-04	I								
Tetrachlorodibenzo-p-dioxin (TCDD), 2,3,7,8-	1746-01-6	1.0E-09	A	1.5E+5	H			3.3E+01	H	1.5E+05	H
Tetrachlorodibenzo-p-dioxins (TCDDs)	41903-57-5			1.5E+05	surr (H)			3.3E+01	surr (H)	1.5E+05	surr (H)
Tetrachlorodibenzofurans (TCDFs)	55722-27-5			1.5E+04	WHO98			3.3E+00	WHO98	1.5E+04	WHO98
Tetrachloroethane, 1,1,2,2-	79-34-5	6.0E-02	SF	2.0E-1	I			5.8E-05	I	2.0E-01	calc
Tetrachloroethane, 1,1,1,2-	630-20-6	3.0E-02	I	2.6E-2	I			7.4E-06	I	2.6E-02	calc
Tetrachloroethylene	127-18-4	1.0E-02	I	5.2E-02	HAD	3.0E-01	A	5.8E-07	HAD	2.0E-03	HAD
Tetrachlorophenol, 2,3,4,6-	58-90-2	3.0E-02	I								
Tetraethyl dithiopyrophosphate (Sulfotep)	3689-24-5	5.0E-04	I								
Thallium	7440-28-0	8.0E-05	surr (I)								
Thiram (Thiuram)	137-26-8	5.0E-03	I								
Toluene	108-88-3	2.0E-01	I			4.0E-01	I				
Toluenediamine, 2,4-	95-80-7			3.2E+00	H			1.1E-03	C99a	3.9E+00	calc
Toluidine, o-	95-53-4			2.4E-1	H			6.9E-05	AC	2.4E-01	AC
Toluidine, p-	106-49-0			1.9E-01	H						
Toxaphene (chlorinated camphenes)	8001-35-2			1.1E+00	I			3.2E-04	I	1.1E+00	calc
Tribromomethane (bromoform)	75-25-2	2.0E-02	I	7.9E-03	I			1.1E-06	I	3.9E-03	calc
Trichloro-1,2,2-trifluoroethane, 1,1,2-	76-13-1	3.0E+01	I			3.0E+01	H				
Trichlorobenzene, 1,2,4-	120-82-1	1.0E-02	I			2.0E-01	H				
Trichloroethane, 1,1,1-	71-55-6	2.8E-01	SF			2.2E+00	SF				

Table 1. Human Health Benchmarks Used in IWEM (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Trichloroethane, 1,1,2-	79-00-5	4.0E-03	I	5.7E-02	I			1.6E-05	I	5.6E-02	calc
Trichloroethylene (1,1,2-trichloroethylene)	79-01-6			1.1E-02	HAD	6.0E-01	C00	1.7E-06	HAD	6.0E-03	HAD
Trichlorofluoromethane (Freon 11)	75-69-4	3.0E-01	I			7.0E-01	H				
Trichlorophenol, 2,4,5-	95-95-4	1.0E-01	I								
Trichlorophenol, 2,4,6-	88-06-2			1.1E-02	I			3.1E-06	I	1.1E-02	calc
Trichlorophenoxy)propionic acid, 2-(2,4,5- (Silvex)	93-72-1	8.0E-03	I								
Trichlorophenoxyacetic acid, 2,4,5-	93-76-5	1.0E-02	I								
Trichloropropane, 1,2,3-	96-18-4	6.0E-03	I	7.0E+00	H	5.0E-03	SF				
Triethylamine	121-44-8					7.0E-03	I				
Trinitrobenzene, sym- (1,3,5-Trinitrobenzene)	99-35-4	3.0E-02	I								
Tris(2,3-dibromopropyl)phosphate	126-72-7			9.8E+00	RQ						
Vanadium	7440-62-2	7.0E-03	H								
Vinyl acetate	108-05-4	1.0E+00	H			2.0E-01	I				
Vinyl chloride	75-01-4	3.0E-03	I	7.2E-01	I	1.0E-01	I	4.4E-06	I	1.5E-02	calc
Xylene, p-	106-42-3	2.0E+00	surr (H)			4.0E-01	surr (A)				
Xylene, m-	108-38-3	2.0E+00	H			4.0E-01	surr (A)				
Xylene, o-	95-47-6	2.0E+00	H			4.0E-01	surr (A)				
Xylenes (total)	1330-20-7	2.0E+00	I			4.0E-01	A				
Zinc	7440-66-6	3.0E-01	I								

Key:

CASRN = Chemical Abstract Service registry number.
RfD = reference dose.
RfC = reference concentration.
CSFo = oral cancer slope factor.
CSFi = inhalation cancer slope factor.
URF = unit risk factor.

Table 1. Human Health Benchmarks Used in IWEM (continued)

[a] Sources:

A	=	ATSDR MRLs (ATSDR, 2001)	I	=	IRIS (U.S. EPA, 2001a)
AC	=	developed for the Air Characteristic Study (U.S. EPA, 1999g)	RQ	=	reportable quantity adjustments (U.S. EPA, 1998d,e,f)
calc	=	calculated	SF	=	Superfund Risk Issue Paper (U.S. EPA, 1998a,b; 1999a,b,c,d,e,f; 2000, 2001b,c,d)
C99a	=	CalEPA cancer potency factor (CalEPA, 1999a)			
C99b	=	CalEPA chronic REL (CalEPA, 1999b)	solv	=	63 FR 64371-0402 (U.S. EPA, 1998c)
C00	=	CalEPA chronic REL (CalEPA, 2000)	surr	=	surrogate (source in parentheses; see section 2.8)
HAD	=	Health Assessment Document (U.S. EPA, 1986a, 1987)	TEF	=	toxicity equivalency factor (U.S. EPA, 1993)
H	=	HEAST (U.S. EPA, 1997)	WHO98	=	World Health Organization (WHO) 1998 toxicity equivalency factor scheme (Van den Berg et al., 1998)

2.4 Dioxin-like Compounds

Cancer slope factors for some dioxin-like compounds were calculated by using the toxic equivalency factor (TEF) approach (Van den Berg et al., 1998). For the TEF approach, the toxicity of a group of chemically related constituents that typically occur in the environment as mixtures is based on estimates of the toxic potency of each constituent as compared with a reference compound within the group. TEF estimates are based on a knowledge of the mechanism of action, available experimental data, and other structure-activity information. TEFs have been established for a number of polychlorinated dibenzodioxins, polychlorinated dibenzofurans, and polychlorinated biphenyl (PCB) congeners thought to have dioxin-like toxicity (Van den Berg et al., 1998). The TEFs listed in Table 2 were used for the dioxin and furan congeners in IWEM.

Table 2. TEFs Used for Dioxin and Furan Congeners

Constituent Name	CASRN	CSFo $(mkd)^{-1}$	CSFo Source	URF $(\mu g/m^3)^{-1}$	URF Source	CSFi $(mkd)^{-1}$	CSFi Source	TEF
Dioxins								
Pentachlorodibenzo-p-dioxin, 1,2,3,7,8-	40321-76-4	1.5E+05	WHO 1998	3.3E+01	WHO 1998	1.5E+05	WHO 1998	1
Tetrachlorodibenzo-p-dioxin, 2,3,7,8-	1746-01-6	1.5E+5	EPA, 1997	3.3E+1	EPA, 1997	1.5E+5	EPA, 1997	1
Hexachlorodibenzo-p-dioxin, 1,2,3,4,7,8-	70648-26-9	1.5E+4	WHO 1998	3.3E+0	WHO 1998	1.5E+4	WHO 1998	0.1
Furans								
Hexachlorodibenzofuran, 1,2,3,4,7,8-	70648-26-9	1.5E+4	WHO 1998	3.3E+0	WHO 1998	1.5E+4	WHO 1998	0.1
Pentachlorodibenzofuran, 2,3,4,7,8-	57117-31-4	7.5E+4	WHO 1998	1.7E+1	WHO 1998	7.5E+4	WHO 1998	0.5
Tetrachlorodibenzofuran, 2,3,7,8-	51207-31-9	1.5E+4	WHO 1998	3.3E+0	WHO 1998	1.5E+4	WHO 1998	0.1

WHO 98 = Van den Berg et al. (1998)
EPA, 1997 = HEAST (U.S. EPA, 1997).

The human health benchmarks calculated using the TEFs for 1,2,3,4,7,8-hexachlorodibenzo-p-dioxin and 1,2,3,4,7,8-hexachlorodibenzofuran were surrogates for hexachlorodibenzo-p-dioxins (HxCDDs) and hexachlorodibenzofurans (HxCDFs), respectively. The human health benchmarks for 1,2,3,7,8-pentachlorodibenzo-p-dioxin and 2,3,4,7,8-pentachlorodibenzofuran were used to represent pentachlorodibenzodioxins (PeCDDs) and pentachlorodibenzofurans (PeCDFs), respectively. The human health benchmarks for 2,3,7,8-tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD) and 2,3,7,8-tetrachlorodibenzofuran were used to represent tetrachlorodibenzo-p-dioxins (TCDDs) and tetrachlorodibenzofurans (TCDFs),

respectively. When TEFs varied within a class of dioxin-like compounds (i.e., pentachlorodibenzofurans), the TEF most protective of human health was used.

2.5 Superfund Technical Support Center Provisional Benchmarks

Table 3 list the provisional human health benchmarks from the Superfund Technical Support Center that were used for some IWEM constituents. A provisional subchronic RfC of 2.0E-2 mg/m^3 was developed by the Superfund Technical Support Center (U.S. EPA, 1999a) for carbon tetrachloride; a provisional chronic RfC of 7.0E-3 mg/m^3 was derived from this value by applying an uncertainty factor of 3 to account for the use of a subchronic study.

Table 3. Provisional Human Health Benchmarks Developed by the Superfund Technical Support Center

CASRN	Chemical Name	Benchmark Type	Benchmark Value	Units	Reference
108-90-7	Chlorobenzene	RfC	6.0E-02	mg/m^3	U.S. EPA, 1998a
7440-48-4	Cobalt (and compounds)	RfD	2.0E-02	mg/kg-d	U.S. EPA, 2001b
100-41-4	Ethylbenzene	URF	1.1E-06	(µg/m3)$^{-1}$	U.S. EPA, 1999b
87-68-3	Hexachlorobutadiene	RfD	3.0E-04	mg/kg-d	U.S. EPA, 1998b
110-54-3	Hexane, n-	RfD	1.1E+01	mg/kg-d	U.S. EPA, 1999c
62-75-9	N-Nitrosodimethylamine (N-methyl-N-nitroso-methanamine)	RfD	8.0E-06	mg/kg-d	U.S. EPA, 2001c
86-30-6	N-Nitrosodiphenylamine	RfD	2.0E-02	mg/kg-d	U.S. EPA, 2001d
79-34-5	Tetrachloroethane, 1,1,2,2-	RfD	6.0E-02	mg/kg-d	U.S. EPA, 2000
71-55-6	Trichloroethane, 1,1,1-	RfD	2.8E-01	mg/kg-d	U.S. EPA, 1999d
71-55-6	Trichloroethane, 1,1,1-	RfC	2.2E+00	mg/m^3	U.S. EPA, 1999e
96-18-4	Trichloropropane, 1,2,3-	RfC	5.0E-03	mg/m^3	U.S. EPA, 1999f

2.6 Benchmarks From Other EPA Sources

For some IWEM constituents, human health benchmarks were not available from IRIS, the Superfund Technical Support Center, HEAST, ATSDR, or CalEPA, but were available from other EPA sources:

- The provisional oral CSF of 5.2E-2 per mg/kg-d, provisional inhalation URF of 5.8E-7 per µg/m^3, and the provisional inhalation CSF of 2.0E-3 per mg/kg-d developed for tetrachloroethylene by EPA in a Health Assessment Document (HAD) (U.S. EPA, 1986a) were used.

- For trichloroethylene, provisional cancer benchmarks developed by EPA in a HAD (U.S. EPA, 1987) were used and include the oral CSF of 1.1E-2 per mg/kg-d, inhalation URF of 1.7E-6 per $\mu g/m^3$, and inhalation CSF of 6.0E-3 per mg/kg-d.

- A provisional RfD of 1.7E-5 mg/kg-d and a provisional RfC of 2.0E-5 mg/m^3 were derived for cyclohexanol in the final listing rule for solvents (63 FR 64371) and were used (U.S. EPA, 1998c).

- An acceptable daily intake (ADI) of 2.0E-03 mg/kg-d from inhalation (7.0E-3 mg/m^3) was identified for pyridine (U.S. EPA, 1986b).

- EPA calculated an oral cancer potency factor of 293 per mg/kg-d for ethyl methanesulfonate in a reportable quantity adjustment evaluation (U.S. EPA, 1998d).

- EPA calculated an oral cancer potency factor of 0.18 per mg/kg-d for safrole in a reportable quantity adjustment evaluation (U.S. EPA, 1998e).

- EPA calculated an oral cancer potency factor of 9.8 per mg/kg-d for tris(2,3-dibromopropyl)phosphate in a reportable quantity adjustment evaluation (U.S. EPA, 1998f).

- The cancer slope factor for dibenzo(a,h)anthracene was calculated by using the TEF approach and a TEF of 1 (U.S. EPA, 1993). The oral CSF for dibenzo(a,h)anthracene was therefore the same as the IRIS (U.S. EPA, 2001a) value for benzo(a)pyrene: 7.3.E+00 $(mg/kg-d)^{-1}$.

2.7 Air Characteristic Study Provisional Benchmarks

Provisional inhalation health benchmarks were developed in the Air Characteristic Study (U.S. EPA, 1999g) for several constituents lacking IRIS, HEAST, alternative EPA, or ATSDR values. For 2-chlorophenol, a provisional RfC was developed using route-to-route extrapolation of the oral RfD. Using route-to-route extrapolations based on oral CSFs from IRIS and HEAST, the Air Characteristic Study developed provisional inhalation URFs and inhalation CSFs for bromodichloromethane, chlorodibromomethane, and o-Toluidine.

These provisional inhalation benchmark values are summarized in Table 4 below. Additional details on the derivation of these inhalation benchmarks can be found in the *Revised Risk Assessment for the Air Characteristic Study* (U.S. EPA, 1999g).

Table 4. Provisional Inhalation Benchmarks Developed in the Air Characteristic Study

CASRN	Chemical Name	RfC (mg/m^3)	RfC Target Effect	URF $(\mu g/m^3)^{-1}$	CSFi $(mg/kg\text{-}d)^{-1}$
75-27-4	Bromodichloromethane (dichlorobromomethane)			1.8E-05	6.2E-02
124-48-1	Chlorodibromomethane (dibromochloromethane)			2.4E-05	8.4E-02
95-57-8	2-Chlorophenol (o-)	1.4E-03	Reproductive, developmental		
95-53-4	o-Toluidine (2-methylaniline)			6.9E-05	2.4E-01

2.8 Surrogate Health Benchmarks

For several IWEM constituents, IRIS benchmarks for similar chemicals were used as surrogate data. The rationale for these recommendations is as follows:

- cis-1,3-Dichloropropylene and trans-1,3-dichloropropylene were based on 1,3-dichloropropene. The studies cited in the IRIS file for 1,3-dichloropropene used a technical-grade chemical that contained about a 50/50 mixture of the cis- and trans-isomers. The RfD is 3E-02 mg/kg-d and the RfC is 2E-02 mg/m^3. The oral CSF for 1,3-dichloropropene is 0.1 $(mg/kg\text{-}d)^{-1}$ and the inhalation URF is 4E-06 $(\mu g/m^3)^{-1}$.

- The IRIS oral CSF for the 2,4-/2,6-dinitrotoluene mixture (6.8E-01 per mg/kg-d) was used as the oral CSFs for 2,4-dinitrotoluene and 2,6-dinitrotoluene.

- The RfDs for o- and m-cresol (both 5E-02 mg/kg/d) are cited on IRIS. The provisional RfD for p-cresol (5E-03 mg/kg/d) is from HEAST. Cresol mixtures contain all three cresol isomers. Based on the hierarchy described above (i.e., IRIS is preferred over HEAST because IRIS is EPA's official repository of Agency-wide consensus human health risk information), the RfD for m-cresol (5E-02 mg/kg-d) was used as a surrogate for cresol mixtures.

- Fluoride was based on fluorine. The IRIS RfD for fluorine (6E-02 mg/kg-d) is based on soluble fluoride.

- The RfD for methyl mercury (1E-04 mg/kg-d) was used as a surrogate for elemental mercury.

- The RfD for Arochlor 1254 (2E-05 mg/kg-d) was used as a surrogate for PCBs.

- Thallium was based on thallium chloride. There are several thallium salts that have RfDs in IRIS. The lowest value among the thallium salts (8E-05 mg/kg-d) is routinely used to represent thallium in risk assessments.

- p-Xylene was based on total xylenes. An RfD of 2 mg/kg-d is listed for total xylenes, m-xylene, and o-xylene in IRIS. Total xylenes contain a mixture of all three isomers; therefore, the RfD likely is appropriate for p-xylene.

2.9 Chloroform

EPA has classified chloroform as a Group B2, Probable Human Carcinogen, based on an increased incidence of several tumor types in rats and mice (U.S. EPA, 2001a). However, based on an evaluation initiated by EPA's Office of Water (OW), the Office of Solid Waste (OSW) now believes the weight of evidence for the carcinogenic mode of action for chloroform does not support a mutagenic mode of action; therefore, a nonlinear low-dose extrapolation is more appropriate for assessing risk from exposure to chloroform. EPA's Science Advisory Board (SAB), the World Health Organization (WHO), the Society of Toxicology, and EPA all strongly endorse the nonlinear approach for assessing risks from chloroform.

Although OW conducted its evaluation of chloroform carcinogenicity for oral exposure, a nonlinear approach for low-dose extrapolation would apply to inhalation exposure to chloroform as well, because chloroform's mode of action is understood to be the same for both ingestion and inhalation exposures. Specifically, tumorigenesis for both ingestion and inhalation exposures is induced through cytotoxicity (cell death) produced by the oxidative generation of highly reactive metabolites (phosgene and hydrochloric acid), followed by regenerative cell proliferation (U.S. EPA, 1998g). Chloroform-induced liver tumors in mice have only been seen after bolus corn oil dosing and have not been observed following administration by other routes (i.e., drinking water and inhalation). As explained in EPA OW's March 31, 1998, and December 16, 1998, *Federal Register* notices pertaining to chloroform (U.S. EPA, 1998g and 1998h, respectively), EPA now believes that "based on the current evidence for the mode of action by which chloroform may cause tumorigenesis, ...a nonlinear approach is more appropriate for extrapolating low-dose cancer risk rather than the low-dose linear approach..."(U.S. EPA, 1998g). OW determined that, given chloroform's mode of carcinogenic action, liver toxicity (a noncancer health effect) actually "is a more sensitive effect of chloroform than the induction of tumors" and that protecting against liver toxicity "should be protective against carcinogenicity given that the putative mode of action understanding for chloroform involves cytotoxicity as a key event preceding tumor development" (U.S. EPA, 1998g).

The recent evaluations conducted by OW concluded that protecting against chloroform's noncancer health effects protects against excess cancer risk. EPA now believes that the noncancer health effects resulting from inhalation of chloroform would precede the development of cancer and would occur at lower doses than would tumor development. Although EPA has not finalized a noncancer health benchmark for inhalation exposure (i.e., an RfC), ATSDR has developed an inhalation MRL for chloroform. Therefore, ATSDR's chronic inhalation MRL for chloroform (0.1 mg/m^3) was used in IWEM.

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Appendix B

Modifications Made to WATER9 to Calculate Sludge Concentrations

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Appendix B
Modifications Made to WATER9 to Calculate Sludge Concentrations

Several modifications to the WATER9 model that are currently under review were used in the Headworks analysis; the model with these modification is referred to as WATER9b. Most of these revisions deal with how sorption to solids is modeled. This appendix describes briefly the modifications to WATER9 to create WATER9b. In addition, Attachment B.1 is the WATER9 documentation of changes to solids sorption calculations from WATER8; this document is included here for the reader's convenience. This attachment has been updated from the existing WATER9 documentation to reflect the WATER9b changes and model validation undertaken for the Headworks analysis, but is otherwise presented as is from the WATER9 documentation.

The primary modification, as it pertains to the Headworks analysis, is the segregation of the interstitial fluid from the solids sorption balance. The currently released version of WATER9 assumes that the solid matter in the wastewater treatment system contains 99 parts water to 1 part solid material. This assumption was made to account for contaminant dissolved in the interstitial fluid of microorganism present in the wastewater. The "solid-to-liquid" phase adsorption coefficient related the concentration of the dissolved liquid phase (mass per volume) to the total mass of contaminant in the cell (both sorbed and dissolved contaminant inside the cell) per mass of solid matter (on a dry basis). This assumption of 99 mass percent water inherent in the wastewater solid limited the utility of the WATER9 model to predict the fate of contaminant when inert solid material (rather than biomass) is present or when sludge dewatering is performed on the biosolids, reducing the water content of the solids stream to below 99 percent.

In both WATER9 and WATER9b versions, solid-liquid partitioning is based on the following equation from Matter-Muller:

$$ksl = 10^{(0.67 \times \log Kow - 2.61)}$$

where

ksl = the partitioning of the compound into biomass solids (g/Kg biomass per g/m3)

K_{ow} = octanol-water partition coefficient (unitless)

WATER9b uses this equation directly to calculate the concentration of contaminant sorbed onto the solids on a dry basis. WATER9 had modified the Matter-Muller equation by adding a 0.099 to ksl, as defined above, so that the partition coefficient specifically includes that mass of contaminant in the interstitial fluid. That is, WATER9 considered the mass sorbed as being the sorbed contaminant plus the dissolved contaminant in the cell per dry weight of cell. This term has been dropped in WATER9b along with ancillary equations to account for the mass sorbed being the mass sorbed the dry matter only (with no correction for interstitial water). These modifications to WATER9 are currently being peer-reviewed, and it is anticipated that the WATER9 modifications used in the Headworks analysis will be publically available in the next release of the WATER9 model.

Attachment B-1

WATER8 and WATER9 Modeling of Tanks and Impoundments

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May 6, 2002

Technical Note

SUBJECT: WATER8 and WATER9 Modeling of Tanks and Impoundments.
FROM: C. Allen, RTI
TO: J. Baskir, RTI

Purpose

This is a memorandum describing the modeling of the fate of a compound in impoundment units and in tank units for the programs WATER8 and WATER9. The scope of the memorandum includes differences between WATER8 and WATER9 in equations that are used for fate modeling, and verification of the identical predictions of compound fate for both WATER8 and WATER9.

This memorandum is organized in the following sections:

Purpose

Summary of relevant changes to modeling approach from WATER8 to WATER9

Summary of verification of WATER9 for cases relevant to the headworks project

a. WATER8/WATER9 comparison for non-sorption components (i.e. showing similarities of WATER8 and WATER9)
b. WATER9 comparison to hand calculations
c. WATER8 to WATER9 comparison for sorption components (i.e. showing differences between WATER8 and WATER9)
   – Chemdat8 nonaerated impoundment
   – Chemdat8 disposal impoundment
d. Material balance (internal check of model)

Documentation of details WATER9 sorption routines

Partitioning of the compound at a unit.
Equation for partitioning in oil
Example calculation of fraction in oil for benzene
Equation for partitioning in solids
Equation for overall partitioning among the four phases
Example calculation of fraction in solids for benzene

Documentation of details of WATER8/WATER9 comparisons

Documentation of details of WATER9/Hand calculations comparisons

Subroutine providing the details of the calculations used by WATER9 for the tank unit
Subroutine providing the details of the calculations used by WATER9 for the impoundment or the lagoon unit
Case 1: Detailed Model Results
Case 2: Detailed Model Results
Case 3: Detailed Model Results

Summary of relevant changes to modeling approach from WATER8 to WATER9

This is primarily a summary of the information that is discussed in detail in the sorption equations documentation, plus other changes relevant to the headworks project.

In the tank unit of WATER9, the following feature was added, relative to WATER8. The storage tank model, as an option, can be modeled as a closed constant level tank if the depth of the tank is set to zero. The quantity of waste processed in the tank is then defined from the flow rate on the inlet waste stream. This option would eliminate the working loss from a closed tank, but would not eliminate the breathing losses.

In WATER8 the sorption of the compounds on biomass, solids, oils, and other material is calculated external to WATER8. The bulk concentration of the wastewater in the unit is calculated, and hand calculations or computer programs are used to estimate the partitioning in the different phases. In WATER9, the concentration of biomass, solids, oils, and water is tracked throughout the system. The biomass is generated in some of the biologically active units, and the solids and oils are added with the waste to the system. The partitioning of the components in these four phases is automatically calculated by WATER9, unlike WATER8.

Additional optional features of WATER9 that are not present in WATER8 include the following:

- Adjustment of Henry's law constant due to partitioning on solids or oils,
- Equilibrium hydrolysis due to pH sensitive ionization, and
- Selective removal of oils or solids from a unit.

Summary of verification of WATER9 for cases relevant to the headworks project

a. WATER8/WATER9 comparison for non-sorption components (i.e. showing similarities of WATER8 and WATER9)

Surface Impoundment or Lagoon Unit		
Case 1 SURFIMP.CDW, a WATER8 distribution file		
Modification(s)	Specified time for emissions, 0.1 months	
Results	WATER8	WATER9
Fraction volatilized	0.1444	0.1444
Fraction biodegraded	0.8528	0.8528
Fraction remaining	0.0028	0.00278

Storage Tank Open		
Case 2 TANKB.CDW, a WATER8 distribution file		
Modification(s)	Contents Mwt, 18 (aqueous waste)	
Results	WATER8	WATER9
Fraction volatilized	0.5549	0.5549
Fraction biodegraded	0.0	0.0
Fraction remaining	0.4451	0.4451

Storage Tank Closed		
Case 3 TANKB.CDW, a WATER8 distribution file		
Modification(s)	Contents Mwt, 18 (aqueous waste)Closed tank	
Results	WATER8	WATER9
Breathing fraction	0.1486	0.1486
Working fraction	0.1663	0.1663
Fraction biodegraded	0.0	0.0
Fraction remaining	0.7098	0.7098

b. WATER9 comparison to hand calculations

The hand calculations are equivalent to the computer calculations of WATER8 and WATER9 for Case 1, Case 2, and Case 3 that are presented in the preceding sections. WATER9 provides a printout of the details of the site-specific calculations for each compound in each unit. This report is important and should be used for site specific verification of the WATER9 calculations for important projects. This report does not always provide full details for some of the intermediate calculations. The reports for Case 1 and Case 2 are edited to provide additional details of the intermediate calculations.

See the section below Documentation of details of WATER9/Hand calculations comparisons for the following information:

The annotated source code with inputs, units of inputs, and actual equations and logic used by WATER9 for calculations.

- A detailed printout of the calculations used for the WATER9 projects: Case 1, Case 2, and Case 3.
- Additional comments and equations to provide additional hand calculation details not automatically provided by WATER9 for Case 1 and Case 3.

c. WATER8 to WATER9 comparison for sorption components (i.e. showing differences between WATER8 and WATER9)

Using the surface impoundment model Case 4, from the file headworks project 2, the overall concentration of benzene exiting the impoundment was 0.96977 g/ M3.

Surface Impoundment		
Case 4: headworks project 2, a WATER9 project file		
Type of unit	Impoundment aqueous waste with 1% solids	
Results	Hand calculation	WATER9b
Fraction effluent benzene in solids	0.406	0.4036
Fraction effluent benzene in water	0.594	0.5963
Concentration in water phase	0.5663	0.5663

The fraction of benzene in the water is 1-fsolids, or 1- 0.4061 = 0.5939. The concentration of the benzene in the aqueous phase is the total concentration, 0.9535 g/ M3 times the overall waste flow rate 0.030 M3/s times the fraction of benzene in the aqueous phase, 0.5939, divided by the flow of water, 0.0297 M3/s, or 0.572 ppmw. The concentration of the benzene in the aqueous phase based upon the total flow (aqueous+solids) is the total concentration in the combined phase, 0.9535 g/ M3 times the fraction of benzene in the aqueous phase, 0.5939, or 0.5663 ppmw.

WATER8 does not estimate the partitioning of the benzene in the surface impoundment. The hand calculation methodology presented here could be used with the WATER8 exit concentrations.

Hand calculations of the above are presented in the section
Example calculation of fraction in solids for benzene

The WATER9 results are presented for Case 4 in the section
Documentation of details of WATER8/WATER9 comparisons

– Chemdat8 nonaerated impoundment
In Chemdat8 the non-aerated impoundment model provided an estimate of sorption on biomass generated in the unit. For sorption considered in Case 1 modified as a flow through impoundment, WATER9 provides partitioning of benzene consistent with Chemdat8 and the nonaerated impoundment.

Flow through Impoundment		
Case 1b: Case 1 modified as a WATER9 project file Surfimp		
Type of unit	Flow through impoundment aqueous waste with 1000 ppm dissolved solids	
Results	Chemdat8	WATER9b
Fraction volatilized	0.121	0.1205
Fraction biologically removed	0.733	0.7305
Fraction sorbed	0.000838	0.00464
Fraction remaining	0.145	0.149

One difference in the above output is that Chemdat8 separates the fraction remaining in the water from the sorbed fraction, and WATER9 includes the sorbed fraction in the reported remaining amount.

– Chemdat8 disposal impoundment
In Chemdat8 the disposal impoundment model provides an estimate of sorption on biomass generated in the unit. For sorption considered in Case 1 modified as a disposal impoundment, WATER9 provides partitioning of benzene similar to Chemdat8 with the disposal impoundment.

Disposal Impoundment		
Case 1b: Case 1 modified as a WATER9 project file Surfimp		
Type of unit	Disposal impoundment aqueous waste with 1000 ppm dissolved solids.	
Results	Chemdat8	WATER9
Fraction volatilized	0.139	0.1383
Fraction biologically removed	0.848	0.8482
Fraction sorbed	0.011	0.0533
Fraction remaining	0.003	0.00822

WATER9 and WATER8 use a very different calculation algorithm for solving for the exit concentration. The Chemdat8 procedure is a direct calculation with an approximation equation, and WATER8/WATER9 use an iterative numerical procedure.

d. Material balance (internal check of model)

The following report provides a material balance on the units in the project file headworks project 2. There was no error reported for the system.

UNIT MATERIAL BALANCE 04-01-2002
BENZENE

Part 1 Balance by unit

No.	in (g/s)	out (g/s)	air,remove (g/s)	sum (g/s)
1 air:	0. E+00	0. E+00	0. E+00	
water	0. E+00	0. E+00	0. E+00	0. E+00
2 air:	0. E+00	0. E+00	2.47 E-04	
water	3. E-02	2.98 E-02	0. E+00	0. E+00
3 air:	0. E+00	0. E+00	0. E+00	
water	1.67 E-02	1.67 E-02	0. E+00	0. E+00
4 air:	0. E+00	0. E+00	1.32 E-04	
water	3. E-02	2.91 E-02	7.75 E-04	-1.46 E-09
5 air:	0. E+00	0. E+00	0. E+00	
water	1.67 E-02	1.67 E-02	0. E+00	0. E+00
6 air:	0. E+00	0. E+00	0. E+00	
water	2.91 E-02	2.91 E-02	0. E+00	0. E+00
7 air:	0. E+00	0. E+00	0. E+00	
water	1.3 E-02	1.3 E-02	0. E+00	0. E+00
TOTAL AIR			3.79 E-04	
TOTAL REMOVAL			7.75 E-04	

Part 2 Overall balance

No.	waste in (g/s)	air (g/s)	remove (g/s)	flow out (g/s)
Loss from open unit surface .00025 g/s.				
2: 34	3. E-02	2.47 E-04	0. E+00	0. E+00
3: 49	0. E+00	0. E+00	0. E+00	0. E+00
Loss from open unit surface .00013 g/s.				
4: 36	3. E-02	1.32 E-04	7.75 E-04	0. E+00
5: 14	0. E+00	0. E+00	0. E+00	1.67 E-02
6: 14	0. E+00	0. E+00	0. E+00	2.91 E-02
7: 14	0. E+00	0. E+00	0. E+00	1.3 E-02
TOTALS		3.79 E-04		7.75 E-04

Total inlet loading of compound from waste 6. E-02 g/s.
Fraction lost to the air .006324
Error in overall material balance -5.1805e-09 g/s
Fraction error in overall material balance .

Documentation of details WATER9 sorption routines

Partitioning of the compound at a unit.

The compound is partitioned into the following four phases in each unit:

- Aqueous phase
- Oil phase
- Solids phase
- Biomass solids phase

Initially the loading of each of these phases is defined by the composition of the waste stream, with the exception of the biomass solids. The biomass solids exiting a unit is defined by the material balance in the unit for the creation of biomass within the unit. The rate of generation of biomass is one half the product of the biomass solids concentrations, the overall biorate, and the amount of dissolved solids.

The sorption of components on solids in WATER9 is currently the same for solids and biomass solids. The organic fraction and the sorption characteristics of solids are not defined in WATER9. If you have special sorption characteristics of the solids, adjust your specifications of the concentrations of the solids concentration in the waste as biomass equivalent solids.

Equation for partitioning in oil

The partitioning into the oil is assumed to be defined by the octanol-water partition coefficient.

$$owr = owpc * oilfract / (1 - oilfract)$$

where:

owr = the oil water ratio, the ratio of the mass in the oil to the mass in the water;
owpc = the octanol-water partition coefficient, the ratio of the concentration in the oil to the concentration in the water; and
oilfract= the fraction of oil present in the wastewater.

Example calculation of fraction in oil for benzene

It is assumed for this calculation that only water and oil are present with a trace amount of benzene, with 9 parts oil to 1 part water.

The benzene octanol water partition coefficient (owpc) is 141.

oilfract =0.9.
owr (g in oil / g in water)= owpc * oilfract / (1 - oilfract)
owr (g in oil / g in water)= 141 * 0.9 / (1 - 0.9)
owr (g in oil / g in water)= 1269
frinoil = owr / (1 + owr) ' frinoil is the fraction in the oil phase
frinoil = 0.99921

Equation for partitioning in solids

The partitioning into the biomass and solids is assumed to be defined by the octanol-water partition coefficient.

$$ksl = 10 ^ (0.67 * low - 2.61)$$

where:

ksl = the partitioning of the compound into biomass solids, (g/Kg biomass per g/m3); and
low = the logarithm base 10 of the octanol-water partition coefficient.
swr = ksl * (solids + biomass) / water

where:

swr = the solids to water ratio, the ratio of the mass in the solids to the mass in the water;
ksl = the partitioning of the compound into biomass solids, (g/Kg biomass per g/m3);
water = the water in the unit (L/s);
solids = the solids in the unit as defined by the waste characteristics (g/s), assumed to have the same sorptive capacity as the biomass; and
biomass = the biomass in the unit (g/s).

Equation for overall partitioning among the four phases

The partitioning into the biomass and solids is assumed to be defined by the octanol-water partition coefficient.

$$\text{Fraction in water} = 1 / (1 + owr + swr)$$

where:

swr = the solids to water ratio, the ratio of the mass in the solids to the mass in the water; and
owr = the oil water ratio, the ratio of the mass in the oil to the mass in the water.

$$\text{Fraction in oil} = owr / (1 + owr + swr)$$

where:
swr = the solids to water ratio, the ratio of the mass in the solids to the mass in the water; and
owr = the oil water ratio, the ratio of the mass in the oil to the mass in the water.

Fraction in solids = swr / (1 + owr + swr) x [solids/(biomass+solids)]

where:
swr = the solids to water ratio, the ratio of the mass in the solids to the mass in the water; and
owr = the oil water ratio, the ratio of the mass in the oil to the mass in the water;
solids = the solids in the unit as defined by the waste characteristics (g/s), assumed to have the same sorptive capacity as the biomass; and
biomass = the biomass in the unit (g/s).

Fraction in biomass = swr / (1 + owr + swr) x [biomass/(biomass+solids)]

where:
swr = the solids to water ratio, the ratio of the mass in the solids to the mass in the water; and
owr = the oil water ratio, the ratio of the mass in the oil to the mass in the water;
solids = the solids in the unit as defined by the waste characteristics (g/s), assumed to have the same sorptive capacity as the biomass; and
biomass = the biomass in the unit (g/s).

If the unit is an API separator then the partitioning into the oil is already defined by the unit calculations; however, the partitioning into the solids may be estimated with the above procedures.

In the case of a lagoon (generally without forced agitation or aeration) the solids and other sorptive material can settle to the base of the lagoon and will not be available for biodegradation, volatilization, or discharge with the components of the waste that remain suspended in the lagoon. A special sorption flag is available to simulate this condition.

Example calculation of fraction in solids for benzene

This example is from the project file: headworks project 2. Benzene is in the impoundment water with a concentration of 0.96977 g/ M3 and a solids concentration of 10000 ppmw. The flow rate of the waste stream is 30 L/s, with a flow of water of 29.7 L/s (99% water, 1% solids). The solids flow rate is 300 g/s for this example.

First ksl, a partitioning factor is estimated from the correlation used by WATER9 for biomass solids.

ksl = 10 ^ (0.67 * low - 2.61)

where:

ksl = the partitioning of the compound into biomass solids, (0.06769 g/Kg biomass per g/m3); and

low = the logarithm base 10 of the octanol-water partition coefficient of benzene, 2.15.

$$swr = ksl * (solids + biomass) / water$$

where:

swr = the solids to water ratio, the ratio of the mass in the solids to the mass in the water 0.6837;

ksl = the partitioning of the compound into biomass solids, (0.06769 g/Kg biomass per g/m3);

water = the water in the unit (29.7 L/s);

solids = the solids in the unit as defined by the waste characteristics (300 g/s), assumed to have the same sorptive capacity as the biomass; and

biomass = the biomass in the unit (0 g/s).

To estimate the fraction of benzene sorbed on the solids, the following equation is used:

$$fsolids = swr / (1 + swr + owr) * solids / (solids + sludge)$$

where:

fsolids = The fraction of benzene that is sorbed on the solids in the waste stream, 0.4061.

swr = the solids to water ratio, the ratio of the mass in the solids to the mass in the water 0.6837;

owr = the oil to water ratio, the ratio of the mass in the oil to the mass in the water 0; there is no oil phase in this example.

solids = the solids in the unit as defined by the waste characteristics (300 g/s), assumed to have the same sorptive capacity as the biomass; and

sludge = the biomass flow rate in the waste stream (0 g/s).

The fraction of benzene in the water is 1-fsolids, or 1- 0.4061 = 0.5939. The concentration of the benzene in the aqueous phase is the total concentration, 0.9535 g/ M3 times the overall waste flow rate 0.030 M3/s times the fraction of benzene in the aqueous phase, 0.5939, divided by the flow of water, 0.0297 M3/s, or 0.572 ppmw. The concentration of the benzene in the aqueous phase based upon the total flow (aqueous+solids) is the total concentration in the combined phase, 0.9535 g/ M3 times the fraction of benzene in the aqueous phase, 0.5939, or 0.5663 ppmw.

This calculation of benzene partitioning may be compared with the WATER9 results presented in the following section. The last line in the following section provides the direct comparison to the hand calculation of 0.5663 ppmw benzene in the aqueous phase.

Documentation of details of WATER8/WATER9 comparisons

The following information provides detailed information about the estimation of benzene sorption onto solids in a surface impoundment. The unit calculations for the lagoon are presented first, followed by WATER9 estimates of the benzene partitioning.

```
          WASTEWATER TREATMENT UNIT  4  05-07-2002
     File  Headworks testrun 2:  BENZENE


Type of unit is lagoon
1 Description of unit                        4     default
2 Wastewater temperature   (C)                     25
3 Length of impoundment (m)                        7.5
4 Depth of impoundment (m)                         2
5 Width of impoundment (m)                         7.5
6 active biomass, impoundment (g/l)                0.05
7 if there is plug flow, enter 1                   0
8 time for emissions in lagoon (months)            0
9 Overall biorate (mg/g bio-hr)                    19
10 sorption flag for solids settling =1            0


COMPOUND PROPERTIES OF BENZENE at 25 deg.C

Type of compound       A8
density  (g/cc)                              0.874
molecular weight                              78.11
diffusion coef. water (cm2/s)                 1.02e-05
diffusion coef. air  (cm2/s)                  0.088
vapor pressure (mm Hg)                        95.26
Henry's law constant (atm-m3/mol)             0.00555   y/x= 308.34
   Reference for Henry's law: Yaws and Yang, 1992 S
vapor pressure temp. coefficients             6.905    1211.033    220.8
The enthalpy of vaporization 90.614 cal/cc.
zero order biorate constant (mg/g-hr)         19.1
first order biorate constant (l/g-hr)         1.4
octanol water partition coefficient           2.15
solubility ppmw 1796.573
UNIFAC code    16:00000000000
CAS code    71-43-2
          The estimated vapor pressure is  95.33174 mm Hg.
DETAILED CALCULATIONS at Unit 4 default
Type: lagoon
COMPOUND: BENZENE
```

```
The oil corrected aqueous HL in the dropping waste stream is 3.083e+02 (y/x)
    Closed or sealed waste drop into the unit._____waste  1 testruns
    Properties of BENZENE at 25. deg.C
       hl= 0.00555 atm-m3/mol      vp= 95.26 mmHg
       k1= 0. L/g-hr          dl= 1.02e-05 cm2/s  dv= 0.088 cm2/s
    The residence time in the unit is 1.0417 hr. (0.0434 days.)
    The fetch to depth ratio (effective width/depth) is 4.2325.
    __Sorption partitioning of component_______
        The fraction sorbed on solids is 0..
       solids fraction sorbed   0.
       biomass fraction sorbed  0.
       oil fraction sorbed      0.
    kg is estimated as 0.00838 m/s.
    Springer correlation does not apply, use Mackay and Yeun (1983).
    The friction velocity is 13.347cm/s.
    The Schmidt number is 980.392.
    kl is estimated as 6.477e-06 m/s.
    Waste rate in the unit 30. (L/s)   0.6848 (MGD)
    concentration into the unit 1. (mg/L)
    compound rate into the unit 0.03 (g/s)   0.2381 (lb/hr)
    compound rate recovered by controls 0. (g/s)   0. (lb/hr)
    fraction recovered by controls 0.
       KG surface (m/s)                          0.00854

       KL surface (m/s)                          6.477e-06

       KL OVERALL SURFACE (m/s)                  6.455e-06

       TOTAL FRACTION VOLATILIZED                0.00685

       FRACTION BIOLOGICALLY REMOVED             0.03965

       FRACTION SUBMERGED VOLATILIZED            0.

       FRACTION ABSORBED                         0.3872

       TOTAL AIR EMISSIONS  (g/s)                0.00021

                        (Mg/year)                0.00648

       EMISSION FACTOR  (g/cm2-s)                3.656e-10

       UNIT EXIT CONCENTRATION (ppmw)            0.5663
```

Documentation of details of WATER9/Hand calculations comparisons

Subroutine providing the details of the calculations used by WATER9 for the tank unit.

```
Sub TANK(nt%)
' edited 3-25-2002
  Call sets8(nt%, n%, ci, Vel, q, temp)
     'n%=number of identical tanks
     'ci=inlet concentration, ppmw.
     'vel=windspeed cm/s
     'q=inlet flow rate m3/s
     'T=temperature in the tank, deg C

'unit inputs _____________________________
 areareal = asgn8(3)
     DENS = asgn8(4)            'g/cc
      mwt = asgn8(5)
storetime = asgn8(6)            'days
       Fp = asgn8(7)            'paint factor
      wid = asgn8(8)            'diameter m
        h = asgn8(9)            'vapor space m
       dt = asgn8(10) * 1.8     'deg F
     AREA = (wid) ^ 2 * 3.141592 / 4 'm2
     le(nt%).AREA = AREA
    depth = asgn8(11)           'm specified as tank height
      vol = depth * AREA        ' m3
 oilfract = asgn8(12) / 100

 'see subroutine fractionoil for details
 If oilfract = 0 Then 'oil fraction not specified, estimated from inflow
    Call fractionoil(oilfract, owpc, owr, frinoil, nt%, hlcor)
 Else
    Call fractionoil(oilfract, owpc, owr, frinoil, 0, hlcor)
 End If
 'oilfraction=fraction of oil in the tank
 'owpc      = oil water partition coefficient
 'owr       = oil water ratio
 'frinoil   = fraction of compound in the oil phase
 'hlcor     = henry's law constant correction for oil partitioning.

 fair = 0: fairs = 0: fairb = 0: fairw = 0

        If storetime = 0 And q = 0 Then
           Exit Sub
        ElseIf storetime = 0 Then
           storetime = vol * n% / q / 3600 / 24
        End If
        If storetime = 0 Then Exit Sub
        qan = n% * ci * vol * DENS / storetime * 365 'g yearly throughput
        If depth = 0 Then
           qan = n% * ci * DENS * q * 24 * 3600 * 365 'g yearly throughput
           If showprint = 1 Then
            pppprnt "The depth in the tank is zero, constant level option."
           End If
        End If
        nturn = 365 / storetime

        Call Tcorr(k1, vmax, dl, dv, vp, Hl, temp, nt%)
        cmwt = aa.mwt: If cmwt = 0 Then cmwt = 80
        If nturn <= 36 Then Kn = 1 Else Kn = (180 + nturn) / 6 / nturn
```

```
        If mwt = 18 Or oilfract = 0 Then 'aqueous
          p = 14.7 * Hl * ci / cmwt * hlcor 'psia
          pmax = vp / 760 * 14.7
          If p > pmax Then p = pmax
          aqueous$ = " Aqueous matrix"
          If showprint = 1 Then ppprnt "The oil corrected aqueous HL is " +
Format$(Hl * hlcor * 55555, "#.###e+00 (y/x)")
          xw = 0
        Else
          coil = ci * frinoil / oilfract
          xw = frinoil * coil / cmwt / (coil / cmwt + (1000000! - coil) / mwt)
          p = xw * vp * 14.7 / 760 'psia
          aqueous$ = " Oily matrix"
        End If
        If p < 0 Then p = 0
        conc = p / 14.7 / 1000000!              'ppmv
        If showprint = 1 Then 'print summary of inputs
            ppprnt "The concentration in the tank inlet is " + Format$(ci,
"#.###e+00 ppmw")
            ppprnt "The flowrate of liquid is " + Format$(q, "#.###e+00") + "
M3/s"
            ppprnt "liquid flowrate (from tank holding) is " + Format$(vol /
storetime / 24 / 3600, "#.###e+00") + " M3/s"
            ppprnt "The total loading of the compound is " + Format$(qan,
"#.##e+00") + " g/yr."
        End If
If areareal > 0 Then 'this section is for an open tank
     If depth = 0 Then depth = 0.3
     fd = wid / depth
     kg = KGC8(Vel, wid * 100, dv, 2)
     kl = KLC8(Vel, fd, dl, temp, 6, 0, 1)
     ko = 1 / (1 / kl + 1 / (Hl * hlcor) / 55555 / kg)
     restime = storetime * 24 * 3600
     Mtr = ko * 0.18 / depth * restime
     fairs = 1 - Exp(-Mtr)
     fair = fairs
     Call setx8(kg, kl, ko, fairs, 0, 0, 0)
Else
'_____calculation of working losses
   If depth = 0 Then 'assumes constant level tank, fixed roof
     fairw = 0
   Else
     G = q * 1000 / 3.75 * 3600 * 24            'gal/day
     v = vol * 1000 / 3.785 'gal
     lw = 0.0000000109 * aa.mwt * p * v * Kn    'Mg/turnover
     If ci > 0 Then fairw = 1000000! * lw / (ci * vol * DENS) Else fairw = 0
     fairw = fairw / (1 + fairw)
     If showprint = 1 Then
            ppprnt "The working volume is " + Format$(vol, "#.###e+00  m3;") +
Format$(v, "#.###e+00  gal")
            ppprnt "The mass lost per turnover is " + Format$(lw, "#.###e+00")
+ " Mg/turnover"
            ppprnt "The vapor pressure of the compound in solution is " +
Format$(p, "#.######") + " psia."
     End If
   End If
'_____calculation of breathing losses
     dia = wid * 3.28    'ft
     h = h * 3.28        'ft
     If dia > 30 Then c = 1 Else c = 0.0771 * dia - 0.0013 * dia ^ 2 - 0.1334
```

```
     Lb2 = 0.0000102 * aa.mwt * (p / (14.7 - p)) ^ 0.68 * dia ^ 1.73
     Lb = n% * Lb2 * h ^ 0.51 * dt ^ 0.5 * Fp * c    'Mg/year
     If qan > 0 Then fairb = 1000000 * Lb / qan Else fairb = 0
  'summary information
     fairb = fairb / (1 + fairb)        'fraction to air from breathing
     fair = fairb + fairw * (1 - fairb) 'total fraction to air
  'printing information_______________
     Call setx8(0, 0, 0, 0, 0, 0, 0)
     If showprint = 1 Then
            ppprnt "MWT = " + Format$(aa.mwt, "###.#") + "    dia= " +
Format$(dia, "####.#  ft.")
            ppprnt "Breathing:  Lb = 0.0000102 * MWT * (p / (14.7 - p)) ^ 0.68
* dia ^ 1.73 "
            ppprnt "mass emissions= Lb * h ^ 0.51 * dt ^ 0.5 * Fp * c   Mg/yr"
            ppprnt "c = " + Format$(c, "#.###") + "    h= " + Format$(h,
"####.#  ft.")
            ppprnt "dt = " + Format$(dt, "##.## ") + "deg.F    Fp= " +
Format$(Fp, "##.###")
            ppprnt "mass emissions= " + Format$(Lb, "##.##E+00 ") + "  Mg/yr"
     End If
 End If

If showprint = 1 Then
  ppprnt "The temperature in the tank is " + Format$(temp, "###.#") + " deg.C"
  ppprnt "The type of liquid is " + aqueous$
  ppprnt "The concentration in the liquid waste is " + Format$(ci, "#.###e+00
g/m3")
  ppprnt "The fraction in the oil is " + Format$(frinoil, "#.#######")
  ppprnt "The vapor pressure (p) is " + Format$(p, "#.###e+00  psia; ") + "("
+ Format$(vp, "#.###e+00  mmHg") + ")"
  ppprnt "The fraction of the compound in oil phase is " + Format$(frinoil,
"#.#####") + "."
  ppprnt "The residence time in the tank is " + Format$(storetime, "###.###")
+ " days."
End If

    Call setx1(storetime, Kn, fairw, fairb, fairs, concg, frinoil, 0, 0, 0)
                   'nt%, fair, fbio, fads, ta, percontrol
    Call sumrates8(nt%, fair, 0, 0, AREA, 0, 0)
    ASGN2(192) = ci * (1 - fair - fbio - fads)

End Sub
```

Subroutine providing the details of the calculations used by WATER9 for the impoundment or the lagoon unit.

```
Sub IMPOUND8(nt%)
    'surface impoundment model
    'input parameters
    Call sets8(nt%, n%, ci, v, q, T)
     'n%=number of impoundments
     'ci=inlet concentration, ppmw.
     'v=windspeed cm/s
     'q=inlet flow rate m3/s
     'T=temperature in the impoundment deg C
    l1 = asgn8(3)       'length, m
    d = asgn8(4)       'depth, m
    If d = 0 Then Exit Sub
    wid = asgn8(5)     'width, m
```

```
    xw = asgn8(6)       'g biomass /l
    If asgn8(7) = 1 Then plugflow = 1
    holdingtime = asgn8(8) 'months. if residence time is specified by waste
flow, set to 0.
    overallbiorate = asgn8(9)
    sorptionflag = asgn8(10)

    AREA = wid * l1      'surface of impoundment m2
    le(nt%).AREA = AREA
    'see subroutine Tcorr for details
    Call Tcorr(k1, vmax, dl, dv, vp, Hl, T, nt%)
    'compound properties adjusted for temperature T(Cel.)
    'k1=first order biorate constant L/g-hr
    'dl, dv diffusion constant liquid and vapor, cm2/s
    'vp vapor pressure mm Hg
    'Hl Henry's law constant atm-m3/mol
    volume = AREA * d   'm3
    dia = Sqr(AREA * 4 / 3.14)  'width m
    If holdingtime > 0 Then 'modified 4-4-02 if q = 0 Then ' model is the same
for either
       plugflow = 1               ' plug flow or disposal
       restime = holdingtime * 365.25 / 12 * 24 'holding time, hr
       checkflowrate holdingtime, volume, q, nt%
       qavg = volume / restime / 3600  'm3/s
       q = qavg
       L(nt%).wflow = q * 1000 'permits only one warning from checkflowrate
       If showprint = 1 Then
         ppprnt "The average flow for specified holding time is
volume/residence time " + FORMP(qavg) + " m3/s. "
       End If
    Else
       restime = l1 * wid * d / q * n% / 3600 'holding time, hr
    End If
    totalin nt%, sumsolids, sumBiomass, sumOil, sumDiss 'g/s
    'sumsolids= solids added to impoundment, g/s average
    'sumbiomass= biomass solids added to impoundment, g/s average
    'sumoil= oil added to impoundment, g/s average
    'sumDiss= dissolved solids added to impoundment, g/s average

    inletsolids = (sumsolids + sumBiomass + sumOil)  'g/s
    fractionsorbed = le(nt%).fsludge + le(nt%).fsolids + le(nt%).foil
    fractionwater = 1 - fractionsorbed
    settle oilremove, solidRemain, waterRemove, solidRemove, nt%
    If le(nt%).cin > 0 Then
       fractionsorbed = (oilremove + solidRemain + waterRemove + solidRemove)
/ le(nt%).cin
       fs2 = (solidRemain + solidRemove) / le(nt%).cin
    Else
       fs2 = 0
       fractionsorbed = 0
    End If
    'add biomass generation
      'g/s  =  gbio/L   mg/gbio-hr    m3      hr/s   L/m3   g/mg
      bioadd = xw * overallbiorate * volume / 3600 * 1000 / 1000 / 2
      'g/s      =  g/s
      maxbioadd = sumDiss / 2
      If bioadd > maxbioadd Then bioadd = maxbioadd * 0.95
      ksl = 10 ^ (0.67 * aa.low - 2.61)     ' g/Kg biomass per g/m3
```

```
    If sorptionflag = 1 Then
      If (sumsolids + sumBiomass) > 0 Then
           fractionbioadd = (le(nt%).fsludge + le(nt%).fsolids) * bioadd /
(sumsolids + sumBiomass)
      Else 'only new biomass

           'kg/m3     = gbio/s   kg/g   m3/s
           If q > 0 Then
             concsolids = bioadd / 1000 / q * n% ' + xb 'kg/M3
             fractionbioadd = ksl * concsolids / (ksl * concsolids + 1)
'assumes solids and oil are similar to biomass
           ElseIf bioadd = 0 Then
             concsolids = 0
             fractionbioadd = 0
           Else
            MsgBox "error in specification for unit " + Str$(nt%)
           End If
      End If
    Else
           fractionsorbed = 0
    End If
    'ld(50).xstart is an internal flag that specifies that Hl is corrected for
sorption
    If ld(50).xstart = 1 Then Hl = Hl * (1 - fractionsorbed) 'sorption
correction of HL
    If bioadd > 0 And maxbioadd > 0 Then le(nt%).Mrds = (bioadd / maxbioadd)
Else le(nt%).Mrds = 0
    le(nt%).bios = bioadd 'g new biomass/s
    fd! = dia / d       'Fetch to depth ratio
    If showprint = 1 Then
        ppprnt "The residence time in the unit is " + FORMP(restime) + " hr.
(" + FORMP(restime / 24) + " days.)"
        If q = 0 Then ppprnt "The residence time was specified."
        ppprnt "The fetch to depth ratio (effective width/depth) is " +
FORMP(fd!) + "."
        If sorptionflag = 1 Then
            ppprnt "The solids are assumed to settle in the lagoon base."
            ppprnt "The fraction sorbed (solids+water) is " +
FORMP(fractionsorbed)
        End If
        ppprnt "__Sorption partitioning of component_______"
        ppprnt "    The fraction sorbed on solids is " + FORMP(fs2) + "."
        sumsolids2 = le(nt%).fsolids + le(nt%).fsludge + le(nt%).foil

        If sumsolids > 0 Then
          ppprnt "   solids fraction sorbed   " + FORMP(fs2 * le(nt%).fsolids
/ sumsolids2)
          ppprnt "   biomass fraction sorbed  " + FORMP(fs2 * le(nt%).fsludge
/ sumsolids2)
          ppprnt "   oil fraction sorbed      " + FORMP(fs2 * le(nt%).foil /
sumsolids2)
        End If
    End If

    'see the details under the functions kgc8, klc8
    kg = KGC8(v, dia * 100, dv, 2)  'gm/c2-s
    kl = KLC8(v, fd!, dl, T, 6, 0, 1)
    ko = 1 / (1 / kl + 1 / Hl / 55555 / kg)
    kair = ko * 0.18 / d * 3600 'hr-1
    If sorptionflag = 1 Then    'solids dropped at base of unit
```

```
       kads = 0                  'not considered when solids drop
    Else                         'solids proceed through system
       '1/hr   gbio/s                  s/hr   kg/g    g/Kg biomass per g/m3
/m3
       kads = (bioadd + inletsolids) * 3600 * 0.001 * ksl / volume  ' /hr
       kads = (1 - fractionwater) / restime / fractionwater '5-7-02
    End If
    kother = kair + kads
    hydrolysisk kother, khydrolysis
    solids = 0
    dissol = 0
    'see the details under the subroutine fract28
    Call fract28(ci * (1 - fractionsorbed), xw, vmax, kother, kair, solids,
dissol, restime, Co, fbio, fair, fraleft, plugflow, 0, fads, cair)

    total = ci * volume 'g in impound

        '__summarize results_______
    If sorptionflag = 1 Then     'solids dropped at base of unit
       fads = 0 'fractionsorbed  'fraction that is adsorbed and not available
for volatilization or biodegradation
    Else                         'solids proceed through system
        If kother > 0 Then
            fdiff = kdiff / kother * fair
            fads = kads / kother * fair
            fhydrolysis = khydrolysis / kother * fair
            fair = kair / kother * fair
        Else: fdiff = 0: fads = 0
        End If
    End If

    fhydrolysis = fhydrolysis * (1 - fractionsorbed)
    fair = fair * (1 - fractionsorbed) 'fraction that is lost to the air
    fdiff = fdiff * (1 - fractionsorbed) 'fraction that is biodegraded
    fbio = fbio * (1 - fractionsorbed) 'fraction that is biodegraded
    fraleft = (1 - fractionsorbed) - fair - fbio - fdiff
    If showprint = 1 And khydrolysis > 0 Then
        ppprnt "  Hydrolysis_____________________________________________"
        ppprnt "The hydrolysis rate is " + FORMP(khydrolysis) + "/hr."
        ppprnt "The fraction removed by hydrolysis is " + FORMP(fhydrolysis)
        ppprnt "The hydrolysis rate is included with the biorate"
        ppprnt "The fraction removed bio without hydrolysis is " + FORMP(fbio)
        fbio = fbio + fhydrolysis
        ppprnt "The fraction removed bio plus hydrolysis is " + FORMP(fbio)
    End If



        '__print results_______
    Call setx8(kg, kl, ko, fair, fbio, fdiff, fads)
    If restime > 0 Then le(nt%).cin = total / restime / 3600 'g/s
    Call sumrates8(nt%, fair, fbio, 0, AREA, 0, fractionsorbed)
    If restime > 0 Then le(nt%).e = total * fair / restime / 3600
    ASGN2(192) = ci * (1 - fair - fbio - fads)
End Sub
```

Case 1: Detailed Model Results

```
            WASTEWATER TREATMENT UNIT  1  04-01-2002
       Disposal impoundment with 1ppmw benzene    BENZENE


     Type of unit is lagoon
     1 Description of unit                        1
     2 Wastewater temperature   (C)                    25
     3 Length of impoundment (m)                       95
     4 Depth of impoundment (m)                        1.8
     5 Width of impoundment (m)                        95
     6 active biomass, impoundment (g/l)               0.05
     7 if there is plug flow, enter 1                  0
     8 time for emissions in lagoon (months)           0.1
     9 Overall biorate (mg/g bio-hr)                   19
     10 sorption flag for solids settling =1           0


     COMPOUND PROPERTIES OF BENZENE at 25 deg.C

     Type of compound       A
     density  (g/cc)                              0.87
     molecular weight                              78.1
     diffusion coef. water (cm2/s)                 9.8e-06
     diffusion coef. air  (cm2/s)                  0.088
     vapor pressure (mm Hg)                        95.2
     Henry's law constant (atm-m3/mol)             0.00555   y/x= 308.34
        Reference for Henry's law: no database value
     vapor pressure temp. coefficients             6.905    1211.033    220.79
     The enthalpy of vaporization 90.218 cal/cc.
     zero order biorate constant (mg/g-hr)         19.
     first order biorate constant (l/g-hr)         1.4
     octanol water partition coefficient           2.15
     solubility ppmw 1780.
     UNIFAC code    16:00000000000
     CAS code    71-43-2
     The estimated vapor pressure is  95.256044 mm Hg.


     DETAILED CALCULATIONS at Unit 1
     Type: lagoon
     COMPOUND: BENZENE


     The residence time was specified as 0.1 month.
     The residence time in the unit is 73.05 hr. (3.0438 days.)


  Estimate the equivalent diameter from the area (95 x 95 m2)
                         dia = Sqr(95*95 * 4 / 3.14)
                                 dia=107.2 m

  kg = 0.00482(v/100)^0.78/(dia)^0.11*(0.000181/0.0012/dv)^-0.67*0.00409

     v     =      447 m/s windspeed
     dia   =      107.22 equivalent length m
     Dv    =      0.088 cm2/s gas diffusivity
     Kg    =      2.6417 e-5 gas mass transfer coefficient gm/c2-s
```

```
    The fetch to depth ratio is 107.22/1.8 = 59.55
Since the fetch to depth ratio is greater than 51.11 Then
      kl = 0.0000002611 * v * v / 10000 * (dl / 0.0000085) ^ 0.66666
      v     =      447 cm/s windspeed
      dl    =      9.8 e-6 cm2/s liquid diffusivity
      Kl    =      3.187 e-5   gm/c2-s liquid mass transfer coefficient

      ko = 1 / (1 / kl + 1 / Hl / 55555 / kg)

      Hl    =      0.00555 atm/(g/m3) Henry's law
      kg    =      2.642 e-5 gm/c2-s gas phase coef.
      Kl    =      3.187 e-5  gm/c2-s liquid phase coef.
      ko    =      3.1743 e-5 gm/c2-s overall mass transfer coef.


      ko is estimated as   (3.1743 e-5)* 0.18 = 5.7146 e-6


      kair = ko * 0.18 / d * 3600

      ko    =      3.1743 e-5 gm/c2-s overall mass transfer
      d     =      1.8 m depth of impoundment
      kair  =      0.011428 hr-1

kads = (bioadd + inletsolids) * 3600 * 0.001 * ksl / volume ' /hr
kads = 0, because bioadd and inletsolids equal 0.

kother = kair + kads
kother = 0.011428 hr-1

WATER8 subroutine
Call fract28(ci * (1 - fractionsorbed), xw, vmax, kother, kair, solids,
dissol, restime, Co, fbio, fair, fraleft, plugflow, 0, fads, cair)

Input values:
     Ci        =   1 g/m3, inlet concentration of benzene
Fractionsorbed =   0
     Xw        =   0.05 biomass, g/L
     vmax      =   19
     kother    =   0.011428 hr-1
     kair      =   0.011428 hr-1
     solids    =   0
     dissol    =   0
     restime   =   73 hr.
     plugflow  =   1 plug flow, because the holding time is specified
     kair      =   0.011428 hr-1

Output values:
     Co        =   0.00278 g/m3
     fbio      =   0.8528
     fair      =   0.14439
     fraleft   =   0.00278
     fads      =   0.0

Details of subroutine

ks = aa.biov / aa.k1
     aa.biov   =   19
     aa.k1     =   1.4
```

```
     ks        =   13.57

An iterative procedure is used to estimate the exit concentration for the
wastewater as it is retained in the basin for the specified 0.1 months.  The
exit concentration c is  0.00278 g/m3.

fbio = (ci - fother - c) / ci
     ci        =   1 g/m3.
     fother    =   0.14439
     c         =   0.00278 g/m3
     fbio      =   0.8528.

fair = kair / kother * fother / ci

     ci        =   1 g/m3.
     kair      =   0.011428 hr-1
     kother    =   0.011428 hr-1
     fother    =   0.14439
     fair      =   0.14439 g/m3.

fads = (1 - ratio) * c / ci
     ratio     =   0.
     fads      =   0

fraleft = c / ci
     ci        =   1 g/m3.
     c         =   0.00278 g/m3
     fraleft   =   0.00278 g/m3.
```

WATER9 summary

KG surface (m/s)	0.00646
KL surface (m/s)	5.736e-06
KL OVERALL SURFACE (m/s)	5.714e-06
TOTAL FRACTION VOLATILIZED	0.1444
FRACTION BIOLOGICALLY REMOVED	0.8528
FRACTION SUBMERGED VOLATILIZED	0.
FRACTION ABSORBED	0.
TOTAL AIR EMISSIONS (g/s)	0.00892
(Mg/year)	0.2813
EMISSION FACTOR (g/cm2-s)	9.883e-11
UNIT EXIT CONCENTRATION (ppmw)	0.00278

Case 2: Detailed Model Results

```
          WASTEWATER TREATMENT UNIT  2  03-25-2002
 Example calculation Section 9.6.3          BENZENE


   Type of unit is storage tank
   1 Description of unit                      2     open storage tank
   2 Wastewater temperature   (C)                   25
   3 Open surface area of tank  (m2)                2
   4 Density of liquid in tank (g/cc)               1
   5 tank waste Mwt, water=18                       18
   6 unit storage time (days)                       8.3
   7 tank paint factor                              1
   8 tank diameter (m)                              5.79
   9 tank vapor space height (m)                    1.37
   10 diurnal temp. change (deg.C)                  11
   11 tank height (m)                               2.7
   12 oil in composite wastewater (wt. %)           0


   COMPOUND PROPERTIES OF BENZENE at 25 deg.C

   Type of compound
   density  (g/cc)                              0.874
   molecular weight                              78.11
   diffusion coef. water (cm2/s)                 9.8e-06
   diffusion coef. air  (cm2/s)                  0.088
   vapor pressure (mm Hg)                        95.26
   Henry's law constant (atm-m3/mol)             0.00555   y/x= 308.33
      Reference for Henry's law: Yaws and Yang, 1992 S
   vapor pressure temp. coefficients             6.905    1211.033    220.8
   The enthalpy of vaporization 90.614 cal/cc.
   zero order biorate constant (mg/g-hr)         19.1
   first order biorate constant (l/g-hr)         1.4
   octanol water partition coefficient           2.13
   solubility ppmw 1790.
   UNIFAC code    16:00000000000
   CAS code    71-43-2
             The estimated vapor pressure is  95.33174 mm Hg.
   DETAILED CALCULATIONS at Unit 2 open storage tank
   Type: storage tank
   COMPOUND: BENZENE

   The oil corrected aqueous HL is 3.083e+02 (y/x)
   The concentration in the tank inlet is 30 ppmw
   The flowrate of liquid is 1.e-04 M3/s
   liquid flowrate (from tank holding) is 9.913e-05 M3/s
   The total loading of the compound is 9.38e+04 g/yr.


Estimate the equivalent diameter is the specified diameter, 5.79 m.

kg = 0.00482(v/100)^0.78/(dia)^0.11*(0.000181/0.0012/dv)^-0.67*0.00409

 v      =    200 cm/s windspeed
 dia    =    5.79 equivalent length m
 Dv     =    0.088 cm2/s gas diffusivity
 Kg     =    1.945 e-5 gas mass transfer coefficient gm/c2-s
```

```
    The fetch to depth ratio is 5.79/2.7 = 2.144
  Since the windspeed (200 cm/s) is less than 350 cm/s, the following
correlation is used.
      kl = 0.00000278 * (dl / 0.0000085) ^ 0.66666

      v    =    200 cm/s windspeed
      dl   =    9.8 e-6 cm2/s liquid diffusivity
      Kl   =    3.057 e-6   gm/c2-s liquid mass transfer coefficient

      ko = 1 / (1 / kl + 1 / Hl / 55555 / kg)

      Hl   =    0.00555 atm/(g/m3) Henry's law
      Kg   =    1.945 e-5 gas mass transfer coefficient gm/c2-s
      Kl   =    3.057 e-6  gm/c2-s liquid phase coef.
      ko   =    1.693 e-5 gm/c2-s overall mass transfer coef.


      ko is estimated as   (1.693 e-5)* 0.18 = 5.7146 e-6 m/s


     restime = STORETIME * 24 * 3600

      storetime    =      8.3 days
      restime      =      717120 sec.

     Mtr = ko * 0.18 / depth * restime * areareal / AREA '4-8-02
      ko    =  1.693 e-5 gm/c2-s overall mass transfer
      d     =  2.7 m depth of liquid
      Mtr   =  0.809552

     fairs = 1 - Exp(-Mtr)

      Mtr   =  0.809552
      fairs =  0.55494


      The temperature in the tank is 25. deg.C
      The type of liquid is  Aqueous matrix

p = 14.7 * Hl * ci / cmwt * hlcor
         ci        =      30 g/m3 inlet concentration of component
         hl        =      0.00555 atm-m3/mol
         cmwt      =      78.11 compound molecular weight
         hlcor     =      1 correction for oil sorption, not needed
         p         =      0.03133   vapor pressure, psia



      The residence time in the tank is 8.3 days.
      Waste rate in the unit 0.1 (L/s)   0.00228 (MGD)
      concentration into the unit 30. (mg/L)
      compound rate into the unit 0.003 (g/s)   0.02381 (lb/hr)
      compound rate recovered by controls 0. (g/s)   0. (lb/hr)
      fraction recovered by controls 0.
         unit storage time (days)                 8.3

         Tank turnover factor                     0.8489
```

Tank working loss (fraction)	0.
Tank breathing loss (fraction)	0.
Open tank volatilization loss	0.5549
concentration in headspace (ppmv)	0.
fraction of compound in oil phase	0.
TOTAL FRACTION VOLATILIZED	0.5549
FRACTION BIOLOGICALLY REMOVED	0.
TOTAL AIR EMISSIONS (g/s)	0.00166
(Mg/year)	0.0525
EMISSION FACTOR (g/cm2-s)	6.323e-09
UNIT EXIT CONCENTRATION (ppmw)	13.352

Case 3: Detailed Model Results

```
        WASTEWATER TREATMENT UNIT  1  04-01-2002
 Example calculation Section 9.6.3          BENZENE


Type of unit is storage tank
1 Description of unit                      1      closed tank
2 Wastewater temperature   (C)                    25
3 Open surface area of tank  (m2)                 0
4 Density of liquid in tank (g/cc)                1
5 tank waste Mwt, water=18                        18
6 unit storage time (days)                        8.3
7 tank paint factor                               1
8 tank diameter (m)                               5.79
9 tank vapor space height (m)                     1.37
10 diurnal temp. change (deg.C)                   11
11 tank height (m)                                2.7
12 oil in composite wastewater (wt. %)            0


COMPOUND PROPERTIES OF BENZENE at 25 deg.C

Type of compound
density  (g/cc)                              0.874
molecular weight                              78.11
diffusion coef. water (cm2/s)                 9.8e-06
diffusion coef. air  (cm2/s)                  0.088
vapor pressure (mm Hg)                        95.26
Henry's law constant (atm-m3/mol)             0.00555   y/x= 308.33
   Reference for Henry's law: Yaws and Yang, 1992 S
vapor pressure temp. coefficients             6.905    1211.033    220.8
The enthalpy of vaporization 90.614 cal/cc.
zero order biorate constant (mg/g-hr)         19.1
first order biorate constant (l/g-hr)         1.4
octanol water partition coefficient           2.13
solubility ppmw 1790.
UNIFAC code    16:00000000000
CAS code    71-43-2
          The estimated vapor pressure is  95.33174 mm Hg.


DETAILED CALCULATIONS at Unit 1  closed tank
Type: storage tank
COMPOUND: BENZENE

Properties of BENZENE at 25. deg.C
   hl= 0.00555 atm-m3/mol      vp= 95.26 mmHg
   k1= 0. L/g-hr          dl= 9.8e-06 cm2/s  dv= 0.088 cm2/s

p = 14.7 * Hl * ci / cmwt * hlcor
         ci        =    30 g/m3 inlet concentration of component
         hl        =    0.00555 atm-m3/mol
         cmwt      =    78.11 compound molecular weight
         hlcor     =    1 correction for oil sorption, not needed
         p         =    0.03133   vapor pressure, psia
```

```
      qan =  ci * vol * DENS / storetime * 365
               ci         =    30 g/m3 inlet concentration of component
               vol =      71.09 m3 tank working volume
               dens       =    1 liquid density g/cc
               storetime= 8.3 days specified retention time in tank
               qan =      93788  g yearly throughput


      nturn = 365 / storetime
               storetime  =    8.3 days specified retention time in tank
               nturn      =    44  number of turnovers in a year


       If nturn <= 36 Then Kn = 1 Else Kn = (180 + nturn) / 6 / nturn
            Kn = (180 + nturn) / 6 / nturn
               nturn      =    44  number of turnovers in a year
               Kn         =    0.8489


     v = vol * 1000 / 3.785 'gal
               vol =      71.09 m3 tank working volume
               v          =    18782   volume working gal

     lw = 0.0000000109 * aa.mwt * p * v * Kn
               v          =    18782   volume working gal
               Kn         =    0.8489
               p          =    0.03133   vapor pressure, psia
               aa.mwt     =    78.11      compound molecular weight
               lw         =    4.2534 e-4   Mg/turnover

     fairw = 1000000! * lw / (ci * vol * DENS)
               ci         =    30 g/m3 inlet concentration of component
               vol =      71.09 m3 tank working volume
               dens       =    1 liquid density g/cc
               lw         =    8.3 days specified retention time in tank
               fairw      =    0.19944  g yearly throughput

fairwc = fairw / (1 + fairw)        'fraction to air from breathing
               fairw      =    0.19944  g yearly throughput
               fairwc     =    0.16628  g yearly throughput




      The concentration in the tank inlet is 30 ppmw
      The flowrate of liquid is 1.e-04 M3/s
      liquid flowrate (from tank holding) is 9.913e-05 M3/s
      The total loading of the compound is 9.38e+04 g/yr.
      The working volume is 7.109e+01  m31.878e+04  gal
      The mass lost per turnover is 4.253e-04 Mg/turnover
      The vapor pressure of the compound in solution is .031335 psia.
      MWT = 78.1    dia= 19.  ft.

    dia = wid * 3.28
               dia =      18.99 diameter, feet
               wid =      5.79 diameter, meters

    hf = h * 3.28
               hf         =    4.494 vapor height,feet
               h          =    1.37 vapor height, meters
```

```
   If dia > 30 Then c = 1 Else c = 0.0771 * dia - 0.0013 * dia ^ 2 - 0.1334
               dia =      18.99 diameter, feet
               c          =    0.8620

    Lb2 = 0.0000102 * mwt * (p / (14.7 - p)) ^ 0.68 * dia ^ 1.73
               p          =    0.03133   vapor pressure, psia
               dia =      18.99 diameter, feet
               mwt =      78.11compound molecular weight
               lb2 =      0.0019831

     Lb =  Lb2 * hf ^ 0.51 * dt ^ 0.5 * Fp * c    'Mg/year
               lb2 =      0.0019831
               hf         =    4.494 vapor height,feet
               dt         =    19.8 diurnal temp. change (deg.F)
                               equals change in temp. deg C x 1.8
               c          =    0.8620
               Fp         =    1 tank paint factor
               Lb         =    0.016368

   fairb = 1000000 * Lb / qan
               Lb         =    0.016368
               qan =      93788 g yearly throughput
               fairb      =    0.17452

   fairbc = fairb / (1 + fairb)        'fraction to air from breathing
                 fairb    =    0.17452
                fairbc    =    0.14859

Overall loss working and breathing
fair = fairb + fairwc * (1 - fairbc)
               fairbc     =    0.14859  fraction working
               fairwc     =    0.16628  fraction breathing
               fair       =    0.29016  fraction breathing plus working
      The temperature in the tank is 25. deg.C
      The type of liquid is  Aqueous matrix
      The concentration in the liquid waste is 30 g/m3
      The fraction in the oil is zero, there is no oil.
      The vapor pressure (p) is 3.133e-02  psia(9.526e+01  mmHg)
      The fraction of the compound in oil phase is ..
      The residence time in the tank is 8.3 days.
      Waste rate in the unit 0.1 (L/s)   0.00228 (MGD)
      concentration into the unit 30. (mg/L)
      compound rate into the unit 0.003 (g/s)   0.02381 (lb/hr)
      compound rate recovered by controls 0. (g/s)   0. (lb/hr)
      fraction recovered by controls 0.

      WATER9 summary for closed top tank
                   unit storage time (days)              8.3
               Tank turnover factor                     0.8489
               Tank working loss (fraction)             0.1663
               Tank breathing loss  (fraction)          0.1486
               Open tank volatilization loss            0.
               TOTAL AIR EMISSIONS  (g/s)               0.00087
                           (Mg/year)         0.02745
            EMISSION FACTOR  (g/cm2-s)              3.306e-09
            UNIT EXIT CONCENTRATION (ppmw)          21.295
```

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Appendix C

Detailed Phase II Groundwater Results

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Table C-1. Adjusted IWEM Protective Concentrations for Risk = 1E-6 and HQ = 1

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Leachate Conc (ppm)	Risk = 1e-6 or HQ = 1			
										Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose		Ingestion	Inhalation	Ingestion	Inhalation
1	Benzene	SI	A	RUN2	CT	CT	CT	CT	2.0E-02	1.2E-01	1.0E-01	8.8E-01	7.8E-01
2	Benzene	SI	D	RUN2	CT	HE	HE	CT	2.0E-02	4.5E-03	4.0E-03	6.2E-03	5.5E-03
3	Benzene	SI	F	RUN2	CT	HE	CT	HE	2.0E-02	8.4E-03	7.5E-03	1.3E-02	1.2E-02
4	Benzene	SI	G	RUN2	CT	CT	HE	HE	2.0E-02	2.7E-02	2.4E-02	1.7E-01	1.5E-01
5	Benzene	SI	B	RUN1	HE	HE	CT	CT	5.1E-02	1.3E-02	1.2E-02	2.1E-02	1.8E-02
6	Benzene	SI	C	RUN1	HE	CT	HE	CT	5.1E-02	4.2E-02	3.7E-02	2.6E-01	2.3E-01
7	Benzene	SI	E	RUN1	HE	CT	CT	HE	5.1E-02	7.5E-02	6.7E-02	5.6E-01	5.0E-01
8	Benzene	SI	B	RUN3	HE	HE	CT	CT	2.3E-01	1.3E-02	1.2E-02	2.1E-02	1.8E-02
9	Benzene	SI	C	RUN3	HE	CT	HE	CT	2.3E-01	4.2E-02	3.7E-02	2.6E-01	2.3E-01
10	Benzene	SI	E	RUN3	HE	CT	CT	HE	2.3E-01	7.5E-02	6.7E-02	5.6E-01	5.0E-01
11	Benzene	SI	B	RUN4	HE	HE	CT	CT	5.4E-01	1.3E-02	1.2E-02	2.1E-02	1.8E-02
12	Benzene	SI	C	RUN4	HE	CT	HE	CT	5.4E-01	4.2E-02	3.7E-02	2.6E-01	2.3E-01
13	Benzene	SI	E	RUN4	HE	CT	CT	HE	5.4E-01	7.5E-02	6.7E-02	5.6E-01	5.0E-01
14	Benzene	SI	B	RUN5	HE	HE	CT	CT	3.1E-02	1.3E-02	1.2E-02	2.1E-02	1.8E-02
15	Benzene	SI	C	RUN5	HE	CT	HE	CT	3.1E-02	4.2E-02	3.7E-02	2.6E-01	2.3E-01
16	Benzene	SI	E	RUN5	HE	CT	CT	HE	3.1E-02	7.5E-02	6.7E-02	5.6E-01	5.0E-01
20	Benzene	Tank	B	RUN1	HE	HE	CT	CT	5.9E-01	1.3E-02	1.2E-02	2.1E-02	1.8E-02
21	Benzene	Tank	C	RUN1	HE	CT	HE	CT	5.9E-01	4.2E-02	3.7E-02	2.6E-01	2.3E-01
22	Benzene	Tank	E	RUN1	HE	CT	CT	HE	5.9E-01	7.5E-02	6.7E-02	5.6E-01	5.0E-01
23	Benzene	Tank	B	RUN3	HE	HE	CT	CT	9.8E-01	1.3E-02	1.2E-02	2.1E-02	1.8E-02

(continued)

Table C-1. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Leachate Conc (ppm)	Risk = 1e-6 or HQ = 1			
										Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose		Ingestion	Inhalation	Ingestion	Inhalation
24	Benzene	Tank	C	RUN3	HE	CT	HE	CT	9.8E-01	4.2E-02	3.7E-02	2.6E-01	2.3E-01
25	Benzene	Tank	E	RUN3	HE	CT	CT	HE	9.8E-01	7.5E-02	6.7E-02	5.6E-01	5.0E-01
26	Benzene	Tank	B	RUN5	HE	HE	CT	CT	3.8E-02	1.3E-02	1.2E-02	2.1E-02	1.8E-02
27	Benzene	Tank	C	RUN5	HE	CT	HE	CT	3.8E-02	4.2E-02	3.7E-02	2.6E-01	2.3E-01
28	Benzene	Tank	E	RUN5	HE	CT	CT	HE	3.8E-02	7.5E-02	6.7E-02	5.6E-01	5.0E-01
29	Benzene	PrimClar	A	RUN7	CT	CT	CT	CT	9.6E-01	1.2E-01	1.0E-01	8.8E-01	7.8E-01
30	Benzene	PrimClar	D	RUN7	CT	HE	HE	CT	9.6E-01	4.5E-03	4.0E-03	6.2E-03	5.5E-03
31	Benzene	PrimClar	F	RUN7	CT	HE	CT	HE	9.6E-01	8.4E-03	7.5E-03	1.3E-02	1.2E-02
32	Benzene	PrimClar	G	RUN7	CT	CT	HE	HE	9.6E-01	2.7E-02	2.4E-02	1.7E-01	1.5E-01
33	Benzene	PrimClar	B	RUN8	HE	HE	CT	CT	9.7E-01	1.3E-02	1.2E-02	2.1E-02	1.8E-02
34	Benzene	PrimClar	C	RUN8	HE	CT	HE	CT	9.7E-01	4.2E-02	3.7E-02	2.6E-01	2.3E-01
35	Benzene	PrimClar	E	RUN8	HE	CT	CT	HE	9.7E-01	7.5E-02	6.7E-02	5.6E-01	5.0E-01
36	Benzene	PrimClar	B	RUN9	HE	HE	CT	CT	9.6E-01	1.3E-02	1.2E-02	2.1E-02	1.8E-02
37	Benzene	PrimClar	C	RUN9	HE	CT	HE	CT	9.6E-01	4.2E-02	3.7E-02	2.6E-01	2.3E-01
38	Benzene	PrimClar	E	RUN9	HE	CT	CT	HE	9.6E-01	7.5E-02	6.7E-02	5.6E-01	5.0E-01
55	Benzene	SecClar	A	RUN7	CT	CT	CT	CT	2.7E-02	1.2E-01	1.0E-01	8.8E-01	7.8E-01
56	Benzene	SecClar	D	RUN7	CT	HE	HE	CT	2.7E-02	4.5E-03	4.0E-03	6.2E-03	5.5E-03
57	Benzene	SecClar	F	RUN7	CT	HE	CT	HE	2.7E-02	8.4E-03	7.5E-03	1.3E-02	1.2E-02
58	Benzene	SecClar	G	RUN7	CT	CT	HE	HE	2.7E-02	2.7E-02	2.4E-02	1.7E-01	1.5E-01
59	Benzene	SecClar	B	RUN8	HE	HE	CT	CT	2.6E-02	1.3E-02	1.2E-02	2.1E-02	1.8E-02
60	Benzene	SecClar	C	RUN8	HE	CT	HE	CT	2.6E-02	4.2E-02	3.7E-02	2.6E-01	2.3E-01

(continued)

Table C-1. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Leachate Conc (ppm)	Risk = 1e-6 or HQ = 1			
										Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose		Ingestion	Inhalation	Ingestion	Inhalation
61	Benzene	SecClar	E	RUN8	HE	CT	CT	HE	2.6E-02	7.5E-02	6.7E-02	5.6E-01	5.0E-01
62	Benzene	SecClar	B	RUN9	HE	HE	CT	CT	5.7E-02	1.3E-02	1.2E-02	2.1E-02	1.8E-02
63	Benzene	SecClar	C	RUN9	HE	CT	HE	CT	5.7E-02	4.2E-02	3.7E-02	2.6E-01	2.3E-01
64	Benzene	SecClar	E	RUN9	HE	CT	CT	HE	5.7E-02	7.5E-02	6.7E-02	5.6E-01	5.0E-01
68	Ethoxyethanol, 2-	SI	A	RUN2	CT	CT	CT	CT	1.9E+00	4.0E+02	1.2E+05	3.1E+03	9.2E+05
69	Ethoxyethanol, 2-	SI	B	RUN1	HE	HE	CT	CT	2.2E+01	4.6E+01	1.4E+04	7.2E+01	2.1E+04
70	Ethoxyethanol, 2-	SI	B	RUN3	HE	HE	CT	CT	2.4E+01	4.6E+01	1.4E+04	7.2E+01	2.1E+04
71	Ethoxyethanol, 2-	SI	B	RUN4	HE	HE	CT	CT	2.2E+01	4.6E+01	1.4E+04	7.2E+01	2.1E+04
72	Ethoxyethanol, 2-	SI	B	RUN5	HE	HE	CT	CT	2.0E+01	4.6E+01	1.4E+04	7.2E+01	2.1E+04
74	Ethoxyethanol, 2-	Tank	B	RUN1	HE	HE	CT	CT	2.5E+01	4.6E+01	1.4E+04	7.2E+01	2.1E+04
75	Ethoxyethanol, 2-	Tank	B	RUN3	HE	HE	CT	CT	2.5E+01	4.6E+01	1.4E+04	7.2E+01	2.1E+04
76	Ethoxyethanol, 2-	Tank	B	RUN5	HE	HE	CT	CT	2.4E+01	4.6E+01	1.4E+04	7.2E+01	2.1E+04
77	Ethoxyethanol, 2-	PrimClar	A	RUN7	CT	CT	CT	CT	2.5E+01	4.0E+02	1.2E+05	3.1E+03	9.2E+05
78	Ethoxyethanol, 2-	PrimClar	B	RUN8	HE	HE	CT	CT	2.5E+01	4.6E+01	1.4E+04	7.2E+01	2.1E+04
79	Ethoxyethanol, 2-	PrimClar	B	RUN9	HE	HE	CT	CT	2.5E+01	4.6E+01	1.4E+04	7.2E+01	2.1E+04
85	Ethoxyethanol, 2-	SecClar	A	RUN7	CT	CT	CT	CT	1.2E+00	4.0E+02	1.2E+05	3.1E+03	9.2E+05
86	Ethoxyethanol, 2-	SecClar	B	RUN8	HE	HE	CT	CT	1.2E+00	4.6E+01	1.4E+04	7.2E+01	2.1E+04
87	Ethoxyethanol, 2-	SecClar	B	RUN9	HE	HE	CT	CT	2.6E+00	4.6E+01	1.4E+04	7.2E+01	2.1E+04
89	Trichloroethane, 1,1,2-	SI	A	RUN2	CT	CT	CT	CT	2.4E-02	7.9E-02	5.1E-02	7.2E-01	4.7E-01
90	Trichloroethane, 1,1,2-	SI	D	RUN2	CT	HE	HE	CT	2.4E-02	2.7E-03	1.8E-03	4.3E-03	2.7E-03
91	Trichloroethane, 1,1,2-	SI	B	RUN1	HE	HE	CT	CT	5.1E-02	7.9E-03	5.1E-03	1.4E-02	9.2E-03

(continued)

Table C-1. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Leachate Conc (ppm)	Risk = 1e-6 or HQ = 1			
										Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose		Ingestion	Inhalation	Ingestion	Inhalation
92	Trichloroethane, 1,1,2-	SI	C	RUN1	HE	CT	HE	CT	5.1E-02	2.9E-02	1.9E-02	2.2E-01	1.4E-01
93	Trichloroethane, 1,1,2-	SI	B	RUN3	HE	HE	CT	CT	2.4E-01	7.9E-03	5.1E-03	1.4E-02	9.2E-03
94	Trichloroethane, 1,1,2-	SI	C	RUN3	HE	CT	HE	CT	2.4E-01	2.9E-02	1.9E-02	2.2E-01	1.4E-01
95	Trichloroethane, 1,1,2-	SI	B	RUN4	HE	HE	CT	CT	6.2E-01	7.9E-03	5.1E-03	1.4E-02	9.2E-03
96	Trichloroethane, 1,1,2-	SI	C	RUN4	HE	CT	HE	CT	6.2E-01	2.9E-02	1.9E-02	2.2E-01	1.4E-01
97	Trichloroethane, 1,1,2-	SI	B	RUN5	HE	HE	CT	CT	3.1E-02	7.9E-03	5.1E-03	1.4E-02	9.2E-03
98	Trichloroethane, 1,1,2-	SI	C	RUN5	HE	CT	HE	CT	3.1E-02	2.9E-02	1.9E-02	2.2E-01	1.4E-01
101	Trichloroethane, 1,1,2-	Tank	B	RUN1	HE	HE	CT	CT	6.0E-01	7.9E-03	5.1E-03	1.4E-02	9.2E-03
102	Trichloroethane, 1,1,2-	Tank	C	RUN1	HE	CT	HE	CT	6.0E-01	2.9E-02	1.9E-02	2.2E-01	1.4E-01
103	Trichloroethane, 1,1,2-	Tank	B	RUN3	HE	HE	CT	CT	9.8E-01	7.9E-03	5.1E-03	1.4E-02	9.2E-03
104	Trichloroethane, 1,1,2-	Tank	C	RUN3	HE	CT	HE	CT	9.8E-01	2.9E-02	1.9E-02	2.2E-01	1.4E-01
105	Trichloroethane, 1,1,2-	Tank	B	RUN5	HE	HE	CT	CT	4.0E-02	7.9E-03	5.1E-03	1.4E-02	9.2E-03
106	Trichloroethane, 1,1,2-	Tank	C	RUN5	HE	CT	HE	CT	4.0E-02	2.9E-02	1.9E-02	2.2E-01	1.4E-01
107	Trichloroethane, 1,1,2-	PrimClar	A	RUN7	CT	CT	CT	CT	9.7E-01	7.9E-02	5.1E-02	7.2E-01	4.7E-01
108	Trichloroethane, 1,1,2-	PrimClar	D	RUN7	CT	HE	HE	CT	9.7E-01	2.7E-03	1.8E-03	4.3E-03	2.7E-03
109	Trichloroethane, 1,1,2-	PrimClar	B	RUN8	HE	HE	CT	CT	9.7E-01	7.9E-03	5.1E-03	1.4E-02	9.2E-03
110	Trichloroethane, 1,1,2-	PrimClar	C	RUN8	HE	CT	HE	CT	9.7E-01	2.9E-02	1.9E-02	2.2E-01	1.4E-01
111	Trichloroethane, 1,1,2-	PrimClar	B	RUN9	HE	HE	CT	CT	9.7E-01	7.9E-03	5.1E-03	1.4E-02	9.2E-03
112	Trichloroethane, 1,1,2-	PrimClar	C	RUN9	HE	CT	HE	CT	9.7E-01	2.9E-02	1.9E-02	2.2E-01	1.4E-01
123	Trichloroethane, 1,1,2-	SecClar	A	RUN7	CT	CT	CT	CT	5.3E-02	7.9E-02	5.1E-02	7.2E-01	4.7E-01
124	Trichloroethane, 1,1,2-	SecClar	D	RUN7	CT	HE	HE	CT	5.3E-02	2.7E-03	1.8E-03	4.3E-03	2.7E-03

(continued)

Table C-1. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Leachate Conc (ppm)	Risk = 1e-6 or HQ = 1			
										Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose		Ingestion	Inhalation	Ingestion	Inhalation
125	Trichloroethane, 1,1,2-	SecClar	B	RUN8	HE	HE	CT	CT	4.8E-02	7.9E-03	5.1E-03	1.4E-02	9.2E-03
126	Trichloroethane, 1,1,2-	SecClar	C	RUN8	HE	CT	HE	CT	4.8E-02	2.9E-02	1.9E-02	2.2E-01	1.4E-01
127	Trichloroethane, 1,1,2-	SecClar	B	RUN9	HE	HE	CT	CT	1.1E-01	7.9E-03	5.1E-03	1.4E-02	9.2E-03
128	Trichloroethane, 1,1,2-	SecClar	C	RUN9	HE	CT	HE	CT	1.1E-01	2.9E-02	1.9E-02	2.2E-01	1.4E-01

Table C-2. Adjusted IWEM Protective Concentrations for Risk = 1E-5

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Leachate Conc (ppm)	Risk = 1E-5			
										Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose		Ingestion	Inhalation	Ingestion	Inhalation
1	Benzene	SI	A	RUN2	CT	CT	CT	CT	2.0E-02	1.2E+00	1.0E+00	8.8E+00	7.8E+00
2	Benzene	SI	D	RUN2	CT	HE	HE	CT	2.0E-02	4.5E-02	4.0E-02	6.2E-02	5.5E-02
3	Benzene	SI	F	RUN2	CT	HE	CT	HE	2.0E-02	8.4E-02	7.5E-02	1.3E-01	1.2E-01
4	Benzene	SI	G	RUN2	CT	CT	HE	HE	2.0E-02	2.7E-01	2.4E-01	1.7E+00	1.5E+00
5	Benzene	SI	B	RUN1	HE	HE	CT	CT	5.1E-02	1.3E-01	1.2E-01	2.1E-01	1.8E-01
6	Benzene	SI	C	RUN1	HE	CT	HE	CT	5.1E-02	4.2E-01	3.7E-01	2.6E+00	2.3E+00
7	Benzene	SI	E	RUN1	HE	CT	CT	HE	5.1E-02	7.5E-01	6.7E-01	5.6E+00	5.0E+00
8	Benzene	SI	B	RUN3	HE	HE	CT	CT	2.3E-01	1.3E-01	1.2E-01	2.1E-01	1.8E-01
9	Benzene	SI	C	RUN3	HE	CT	HE	CT	2.3E-01	4.2E-01	3.7E-01	2.6E+00	2.3E+00
10	Benzene	SI	E	RUN3	HE	CT	CT	HE	2.3E-01	7.5E-01	6.7E-01	5.6E+00	5.0E+00
11	Benzene	SI	B	RUN4	HE	HE	CT	CT	5.4E-01	1.3E-01	1.2E-01	2.1E-01	1.8E-01
12	Benzene	SI	C	RUN4	HE	CT	HE	CT	5.4E-01	4.2E-01	3.7E-01	2.6E+00	2.3E+00
13	Benzene	SI	E	RUN4	HE	CT	CT	HE	5.4E-01	7.5E-01	6.7E-01	5.6E+00	5.0E+00
14	Benzene	SI	B	RUN5	HE	HE	CT	CT	3.1E-02	1.3E-01	1.2E-01	2.1E-01	1.8E-01
15	Benzene	SI	C	RUN5	HE	CT	HE	CT	3.1E-02	4.2E-01	3.7E-01	2.6E+00	2.3E+00
16	Benzene	SI	E	RUN5	HE	CT	CT	HE	3.1E-02	7.5E-01	6.7E-01	5.6E+00	5.0E+00
20	Benzene	Tank	B	RUN1	HE	HE	CT	CT	5.9E-01	1.3E-01	1.2E-01	2.1E-01	1.8E-01
21	Benzene	Tank	C	RUN1	HE	CT	HE	CT	5.9E-01	4.2E-01	3.7E-01	2.6E+00	2.3E+00
22	Benzene	Tank	E	RUN1	HE	CT	CT	HE	5.9E-01	7.5E-01	6.7E-01	5.6E+00	5.0E+00
23	Benzene	Tank	B	RUN3	HE	HE	CT	CT	9.8E-01	1.3E-01	1.2E-01	2.1E-01	1.8E-01
24	Benzene	Tank	C	RUN3	HE	CT	HE	CT	9.8E-01	4.2E-01	3.7E-01	2.6E+00	2.3E+00

(continued)

Table C-2. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Leachate Conc (ppm)	Risk = 1E-5			
										Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose		Ingestion	Inhalation	Ingestion	Inhalation
25	Benzene	Tank	E	RUN3	HE	CT	CT	HE	9.8E-01	7.5E-01	6.7E-01	5.6E+00	5.0E+00
26	Benzene	Tank	B	RUN5	HE	HE	CT	CT	3.8E-02	1.3E-01	1.2E-01	2.1E-01	1.8E-01
27	Benzene	Tank	C	RUN5	HE	CT	HE	CT	3.8E-02	4.2E-01	3.7E-01	2.6E+00	2.3E+00
28	Benzene	Tank	E	RUN5	HE	CT	CT	HE	3.8E-02	7.5E-01	6.7E-01	5.6E+00	5.0E+00
29	Benzene	PrimClar	A	RUN7	CT	CT	CT	CT	9.6E-01	1.2E+00	1.0E+00	8.8E+00	7.8E+00
30	Benzene	PrimClar	D	RUN7	CT	HE	HE	CT	9.6E-01	4.5E-02	4.0E-02	6.2E-02	5.5E-02
31	Benzene	PrimClar	F	RUN7	CT	HE	CT	HE	9.6E-01	8.4E-02	7.5E-02	1.3E-01	1.2E-01
32	Benzene	PrimClar	G	RUN7	CT	CT	HE	HE	9.6E-01	2.7E-01	2.4E-01	1.7E+00	1.5E+00
33	Benzene	PrimClar	B	RUN8	HE	HE	CT	CT	9.7E-01	1.3E-01	1.2E-01	2.1E-01	1.8E-01
34	Benzene	PrimClar	C	RUN8	HE	CT	HE	CT	9.7E-01	4.2E-01	3.7E-01	2.6E+00	2.3E+00
35	Benzene	PrimClar	E	RUN8	HE	CT	CT	HE	9.7E-01	7.5E-01	6.7E-01	5.6E+00	5.0E+00
36	Benzene	PrimClar	B	RUN9	HE	HE	CT	CT	9.6E-01	1.3E-01	1.2E-01	2.1E-01	1.8E-01
37	Benzene	PrimClar	C	RUN9	HE	CT	HE	CT	9.6E-01	4.2E-01	3.7E-01	2.6E+00	2.3E+00
38	Benzene	PrimClar	E	RUN9	HE	CT	CT	HE	9.6E-01	7.5E-01	6.7E-01	5.6E+00	5.0E+00
55	Benzene	SecClar	A	RUN7	CT	CT	CT	CT	2.7E-02	1.2E+00	1.0E+00	8.8E+00	7.8E+00
56	Benzene	SecClar	D	RUN7	CT	HE	HE	CT	2.7E-02	4.5E-02	4.0E-02	6.2E-02	5.5E-02
57	Benzene	SecClar	F	RUN7	CT	HE	CT	HE	2.7E-02	8.4E-02	7.5E-02	1.3E-01	1.2E-01
58	Benzene	SecClar	G	RUN7	CT	CT	HE	HE	2.7E-02	2.7E-01	2.4E-01	1.7E+00	1.5E+00
59	Benzene	SecClar	B	RUN8	HE	HE	CT	CT	2.6E-02	1.3E-01	1.2E-01	2.1E-01	1.8E-01
60	Benzene	SecClar	C	RUN8	HE	CT	HE	CT	2.6E-02	4.2E-01	3.7E-01	2.6E+00	2.3E+00
61	Benzene	SecClar	E	RUN8	HE	CT	CT	HE	2.6E-02	7.5E-01	6.7E-01	5.6E+00	5.0E+00
62	Benzene	SecClar	B	RUN9	HE	HE	CT	CT	5.7E-02	1.3E-01	1.2E-01	2.1E-01	1.8E-01
63	Benzene	SecClar	C	RUN9	HE	CT	HE	CT	5.7E-02	4.2E-01	3.7E-01	2.6E+00	2.3E+00

(continued)

Table C-2. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Leachate Conc (ppm)	Risk = 1E-5			
										Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose		Ingestion	Inhalation	Ingestion	Inhalation
64	Benzene	SecClar	E	RUN9	HE	CT	CT	HE	5.7E-02	7.5E-01	6.7E-01	5.6E+00	5.0E+00
89	Trichloroethane, 1,1,2-	SI	A	RUN2	CT	CT	CT	CT	2.4E-02	7.9E-01	5.1E-01	7.2E+00	4.7E+00
90	Trichloroethane, 1,1,2-	SI	D	RUN2	CT	HE	HE	CT	2.4E-02	2.7E-02	1.8E-02	4.3E-02	2.7E-02
91	Trichloroethane, 1,1,2-	SI	B	RUN1	HE	HE	CT	CT	5.1E-02	7.9E-02	5.1E-02	1.4E-01	9.2E-02
92	Trichloroethane, 1,1,2-	SI	C	RUN1	HE	CT	HE	CT	5.1E-02	2.9E-01	1.9E-01	2.2E+00	1.4E+00
93	Trichloroethane, 1,1,2-	SI	B	RUN3	HE	HE	CT	CT	2.4E-01	7.9E-02	5.1E-02	1.4E-01	9.2E-02
94	Trichloroethane, 1,1,2-	SI	C	RUN3	HE	CT	HE	CT	2.4E-01	2.9E-01	1.9E-01	2.2E+00	1.4E+00
95	Trichloroethane, 1,1,2-	SI	B	RUN4	HE	HE	CT	CT	6.2E-01	7.9E-02	5.1E-02	1.4E-01	9.2E-02
96	Trichloroethane, 1,1,2-	SI	C	RUN4	HE	CT	HE	CT	6.2E-01	2.9E-01	1.9E-01	2.2E+00	1.4E+00
97	Trichloroethane, 1,1,2-	SI	B	RUN5	HE	HE	CT	CT	3.1E-02	7.9E-02	5.1E-02	1.4E-01	9.2E-02
98	Trichloroethane, 1,1,2-	SI	C	RUN5	HE	CT	HE	CT	3.1E-02	2.9E-01	1.9E-01	2.2E+00	1.4E+00
101	Trichloroethane, 1,1,2-	Tank	B	RUN1	HE	HE	CT	CT	6.0E-01	7.9E-02	5.1E-02	1.4E-01	9.2E-02
102	Trichloroethane, 1,1,2-	Tank	C	RUN1	HE	CT	HE	CT	6.0E-01	2.9E-01	1.9E-01	2.2E+00	1.4E+00
103	Trichloroethane, 1,1,2-	Tank	B	RUN3	HE	HE	CT	CT	9.8E-01	7.9E-02	5.1E-02	1.4E-01	9.2E-02
104	Trichloroethane, 1,1,2-	Tank	C	RUN3	HE	CT	HE	CT	9.8E-01	2.9E-01	1.9E-01	2.2E+00	1.4E+00
105	Trichloroethane, 1,1,2-	Tank	B	RUN5	HE	HE	CT	CT	4.0E-02	7.9E-02	5.1E-02	1.4E-01	9.2E-02
106	Trichloroethane, 1,1,2-	Tank	C	RUN5	HE	CT	HE	CT	4.0E-02	2.9E-01	1.9E-01	2.2E+00	1.4E+00
107	Trichloroethane, 1,1,2-	PrimClar	A	RUN7	CT	CT	CT	CT	9.7E-01	7.9E-01	5.1E-01	7.2E+00	4.7E+00
108	Trichloroethane, 1,1,2-	PrimClar	D	RUN7	CT	HE	HE	CT	9.7E-01	2.7E-02	1.8E-02	4.3E-02	2.7E-02
109	Trichloroethane, 1,1,2-	PrimClar	B	RUN8	HE	HE	CT	CT	9.7E-01	7.9E-02	5.1E-02	1.4E-01	9.2E-02
110	Trichloroethane, 1,1,2-	PrimClar	C	RUN8	HE	CT	HE	CT	9.7E-01	2.9E-01	1.9E-01	2.2E+00	1.4E+00
111	Trichloroethane, 1,1,2-	PrimClar	B	RUN9	HE	HE	CT	CT	9.7E-01	7.9E-02	5.1E-02	1.4E-01	9.2E-02
112	Trichloroethane, 1,1,2-	PrimClar	C	RUN9	HE	CT	HE	CT	9.7E-01	2.9E-01	1.9E-01	2.2E+00	1.4E+00

(continued)

Table C-2. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Leachate Conc (ppm)	Risk = 1E-5			
										Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose		Ingestion	Inhalation	Ingestion	Inhalation
123	Trichloroethane, 1,1,2-	SecClar	A	RUN7	CT	CT	CT	CT	5.3E-02	7.9E-01	5.1E-01	7.2E+00	4.7E+00
124	Trichloroethane, 1,1,2-	SecClar	D	RUN7	CT	HE	HE	CT	5.3E-02	2.7E-02	1.8E-02	4.3E-02	2.7E-02
125	Trichloroethane, 1,1,2-	SecClar	B	RUN8	HE	HE	CT	CT	4.8E-02	7.9E-02	5.1E-02	1.4E-01	9.2E-02
126	Trichloroethane, 1,1,2-	SecClar	C	RUN8	HE	CT	HE	CT	4.8E-02	2.9E-01	1.9E-01	2.2E+00	1.4E+00
127	Trichloroethane, 1,1,2-	SecClar	B	RUN9	HE	HE	CT	CT	1.1E-01	7.9E-02	5.1E-02	1.4E-01	9.2E-02
128	Trichloroethane, 1,1,2-	SecClar	C	RUN9	HE	CT	HE	CT	1.1E-01	2.9E-01	1.9E-01	2.2E+00	1.4E+00

NA = not applicable. For 2-ethoxyethanol, only values for HQ =1 were calculated, and these are shown in Table C-1.

Table C-3. Ratio of Leachate Concentration to Adjusted IWEM Protective Concentration for Risk = 1E-6 or HQ = 1

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Risk = 1E-6 or HQ = 1			
									Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose	Ingestion	Inhalation	Ingestion	Inhalation
1	Benzene	SI	A	RUN2	CT	CT	CT	CT	1.7E-01	1.9E-01	2.2E-02	2.5E-02
2	Benzene	SI	D	RUN2	CT	HE	HE	CT	4.4E+00	4.9E+00	3.2E+00	3.6E+00
3	Benzene	SI	F	RUN2	CT	HE	CT	HE	2.3E+00	2.6E+00	1.5E+00	1.7E+00
4	Benzene	SI	G	RUN2	CT	CT	HE	HE	7.3E-01	8.3E-01	1.2E-01	1.3E-01
5	Benzene	SI	B	RUN1	HE	HE	CT	CT	3.8E+00	4.3E+00	2.4E+00	2.8E+00
6	Benzene	SI	C	RUN1	HE	CT	HE	CT	1.2E+00	1.4E+00	1.9E-01	2.2E-01
7	Benzene	SI	E	RUN1	HE	CT	CT	HE	6.7E-01	7.6E-01	9.0E-02	1.0E-01
8	Benzene	SI	B	RUN3	HE	HE	CT	CT	1.8E+01	2.0E+01	1.1E+01	1.3E+01
9	Benzene	SI	C	RUN3	HE	CT	HE	CT	5.5E+00	6.3E+00	8.8E-01	1.0E+00
10	Benzene	SI	E	RUN3	HE	CT	CT	HE	3.1E+00	3.5E+00	4.2E-01	4.7E-01
11	Benzene	SI	B	RUN4	HE	HE	CT	CT	4.1E+01	4.7E+01	2.6E+01	3.0E+01
12	Benzene	SI	C	RUN4	HE	CT	HE	CT	1.3E+01	1.5E+01	2.1E+00	2.3E+00
13	Benzene	SI	E	RUN4	HE	CT	CT	HE	7.2E+00	8.1E+00	9.7E-01	1.1E+00
14	Benzene	SI	B	RUN5	HE	HE	CT	CT	2.3E+00	2.7E+00	1.5E+00	1.7E+00
15	Benzene	SI	C	RUN5	HE	CT	HE	CT	7.3E-01	8.3E-01	1.2E-01	1.3E-01
16	Benzene	SI	E	RUN5	HE	CT	CT	HE	4.1E-01	4.6E-01	5.5E-02	6.2E-02
20	Benzene	Tank	B	RUN1	HE	HE	CT	CT	NA	NA	2.9E+01	3.2E+01
21	Benzene	Tank	C	RUN1	HE	CT	HE	CT	NA	NA	2.2E+00	2.5E+00
22	Benzene	Tank	E	RUN1	HE	CT	CT	HE	NA	NA	1.1E+00	1.2E+00
23	Benzene	Tank	B	RUN3	HE	HE	CT	CT	NA	NA	4.7E+01	5.4E+01
24	Benzene	Tank	C	RUN3	HE	CT	HE	CT	NA	NA	3.7E+00	4.2E+00

(continued)

Table C-3. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Risk = 1E-6 or HQ = 1			
									Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose	Ingestion	Inhalation	Ingestion	Inhalation
25	Benzene	Tank	E	RUN3	HE	CT	CT	HE	NA	NA	1.7E+00	2.0E+00
26	Benzene	Tank	B	RUN5	HE	HE	CT	CT	NA	NA	1.8E+00	2.1E+00
27	Benzene	Tank	C	RUN5	HE	CT	HE	CT	NA	NA	1.4E-01	1.6E-01
28	Benzene	Tank	E	RUN5	HE	CT	CT	HE	NA	NA	6.7E-02	7.6E-02
29	Benzene	PrimClar	A	RUN7	CT	CT	CT	CT	NA	NA	1.1E+00	1.2E+00
30	Benzene	PrimClar	D	RUN7	CT	HE	HE	CT	NA	NA	1.6E+02	1.8E+02
31	Benzene	PrimClar	F	RUN7	CT	HE	CT	HE	NA	NA	7.3E+01	8.2E+01
32	Benzene	PrimClar	G	RUN7	CT	CT	HE	HE	NA	NA	5.7E+00	6.4E+00
33	Benzene	PrimClar	B	RUN8	HE	HE	CT	CT	NA	NA	4.7E+01	5.3E+01
34	Benzene	PrimClar	C	RUN8	HE	CT	HE	CT	NA	NA	3.7E+00	4.1E+00
35	Benzene	PrimClar	E	RUN8	HE	CT	CT	HE	NA	NA	1.7E+00	1.9E+00
36	Benzene	PrimClar	B	RUN9	HE	HE	CT	CT	NA	NA	4.7E+01	5.3E+01
37	Benzene	PrimClar	C	RUN9	HE	CT	HE	CT	NA	NA	3.7E+00	4.1E+00
38	Benzene	PrimClar	E	RUN9	HE	CT	CT	HE	NA	NA	1.7E+00	1.9E+00
55	Benzene	SecClar	A	RUN7	CT	CT	CT	CT	2.3E-01	2.6E-01	3.0E-02	3.4E-02
56	Benzene	SecClar	D	RUN7	CT	HE	HE	CT	5.9E+00	6.7E+00	4.3E+00	4.9E+00
57	Benzene	SecClar	F	RUN7	CT	HE	CT	HE	3.2E+00	3.6E+00	2.0E+00	2.3E+00
58	Benzene	SecClar	G	RUN7	CT	CT	HE	HE	1.0E+00	1.1E+00	1.6E-01	1.8E-01
59	Benzene	SecClar	B	RUN8	HE	HE	CT	CT	1.9E+00	2.2E+00	1.2E+00	1.4E+00
60	Benzene	SecClar	C	RUN8	HE	CT	HE	CT	6.1E-01	6.9E-01	9.7E-02	1.1E-01
61	Benzene	SecClar	E	RUN8	HE	CT	CT	HE	3.4E-01	3.8E-01	4.6E-02	5.1E-02
62	Benzene	SecClar	B	RUN9	HE	HE	CT	CT	4.3E+00	4.9E+00	2.7E+00	3.1E+00
63	Benzene	SecClar	C	RUN9	HE	CT	HE	CT	1.3E+00	1.5E+00	2.1E-01	2.4E-01

(continued)

Table C-3. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Risk = 1E-6 or HQ = 1			
									Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose	Ingestion	Inhalation	Ingestion	Inhalation
64	Benzene	SecClar	E	RUN9	HE	CT	CT	HE	7.6E-01	8.5E-01	1.0E-01	1.1E-01
68	Ethoxyethanol, 2-	SI	A	RUN2	CT	CT	CT	CT	4.7E-03	1.6E-05	6.0E-04	2.0E-06
69	Ethoxyethanol, 2-	SI	B	RUN1	HE	HE	CT	CT	4.7E-01	1.6E-03	3.0E-01	1.0E-03
70	Ethoxyethanol, 2-	SI	B	RUN3	HE	HE	CT	CT	5.3E-01	1.8E-03	3.4E-01	1.1E-03
71	Ethoxyethanol, 2-	SI	B	RUN4	HE	HE	CT	CT	4.7E-01	1.6E-03	3.0E-01	1.0E-03
72	Ethoxyethanol, 2-	SI	B	RUN5	HE	HE	CT	CT	4.3E-01	1.4E-03	2.7E-01	9.2E-04
74	Ethoxyethanol, 2-	Tank	B	RUN1	HE	HE	CT	CT	NA	NA	3.5E-01	1.2E-03
75	Ethoxyethanol, 2-	Tank	B	RUN3	HE	HE	CT	CT	NA	NA	3.5E-01	1.2E-03
76	Ethoxyethanol, 2-	Tank	B	RUN5	HE	HE	CT	CT	NA	NA	3.4E-01	1.1E-03
77	Ethoxyethanol, 2-	PrimClar	A	RUN7	CT	CT	CT	CT	NA	NA	8.0E-03	2.7E-05
78	Ethoxyethanol, 2-	PrimClar	B	RUN8	HE	HE	CT	CT	NA	NA	3.5E-01	1.2E-03
79	Ethoxyethanol, 2-	PrimClar	B	RUN9	HE	HE	CT	CT	NA	NA	3.5E-01	1.2E-03
85	Ethoxyethanol, 2-	SecClar	A	RUN7	CT	CT	CT	CT	2.9E-03	9.9E-06	3.8E-04	1.3E-06
86	Ethoxyethanol, 2-	SecClar	B	RUN8	HE	HE	CT	CT	2.5E-02	8.5E-05	1.6E-02	5.4E-05
87	Ethoxyethanol, 2-	SecClar	B	RUN9	HE	HE	CT	CT	5.6E-02	1.9E-04	3.6E-02	1.2E-04
89	Trichloroethane, 1,1,2-	SI	A	RUN2	CT	CT	CT	CT	3.0E-01	4.7E-01	3.3E-02	5.2E-02
90	Trichloroethane, 1,1,2-	SI	D	RUN2	CT	HE	HE	CT	8.8E+00	1.4E+01	5.6E+00	8.7E+00
91	Trichloroethane, 1,1,2-	SI	B	RUN1	HE	HE	CT	CT	6.5E+00	1.0E+01	3.6E+00	5.6E+00
92	Trichloroethane, 1,1,2-	SI	C	RUN1	HE	CT	HE	CT	1.8E+00	2.8E+00	2.4E-01	3.7E-01
93	Trichloroethane, 1,1,2-	SI	B	RUN3	HE	HE	CT	CT	3.0E+01	4.6E+01	1.7E+01	2.6E+01
94	Trichloroethane, 1,1,2-	SI	C	RUN3	HE	CT	HE	CT	8.3E+00	1.3E+01	1.1E+00	1.7E+00
95	Trichloroethane, 1,1,2-	SI	B	RUN4	HE	HE	CT	CT	7.8E+01	1.2E+02	4.4E+01	6.8E+01
96	Trichloroethane, 1,1,2-	SI	C	RUN4	HE	CT	HE	CT	2.2E+01	3.3E+01	2.9E+00	4.4E+00

(continued)

Table C-3. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Risk = 1E-6 or HQ = 1			
									Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose	Ingestion	Inhalation	Ingestion	Inhalation
97	Trichloroethane, 1,1,2-	SI	B	RUN5	HE	HE	CT	CT	4.0E+00	6.1E+00	2.2E+00	3.4E+00
98	Trichloroethane, 1,1,2-	SI	C	RUN5	HE	CT	HE	CT	1.1E+00	1.7E+00	1.5E-01	2.2E-01
101	Trichloroethane, 1,1,2-	Tank	B	RUN1	HE	HE	CT	CT	NA	NA	4.2E+01	6.5E+01
102	Trichloroethane, 1,1,2-	Tank	C	RUN1	HE	CT	HE	CT	NA	NA	2.8E+00	4.3E+00
103	Trichloroethane, 1,1,2-	Tank	B	RUN3	HE	HE	CT	CT	NA	NA	6.9E+01	1.1E+02
104	Trichloroethane, 1,1,2-	Tank	C	RUN3	HE	CT	HE	CT	NA	NA	4.6E+00	7.0E+00
105	Trichloroethane, 1,1,2-	Tank	B	RUN5	HE	HE	CT	CT	NA	NA	2.8E+00	4.3E+00
106	Trichloroethane, 1,1,2-	Tank	C	RUN5	HE	CT	HE	CT	NA	NA	1.8E-01	2.8E-01
107	Trichloroethane, 1,1,2-	PrimClar	A	RUN7	CT	CT	CT	CT	NA	NA	1.3E+00	2.1E+00
108	Trichloroethane, 1,1,2-	PrimClar	D	RUN7	CT	HE	HE	CT	NA	NA	2.3E+02	3.5E+02
109	Trichloroethane, 1,1,2-	PrimClar	B	RUN8	HE	HE	CT	CT	NA	NA	6.9E+01	1.1E+02
110	Trichloroethane, 1,1,2-	PrimClar	C	RUN8	HE	CT	HE	CT	NA	NA	4.5E+00	7.0E+00
111	Trichloroethane, 1,1,2-	PrimClar	B	RUN9	HE	HE	CT	CT	NA	NA	6.8E+01	1.1E+02
112	Trichloroethane, 1,1,2-	PrimClar	C	RUN9	HE	CT	HE	CT	NA	NA	4.5E+00	6.9E+00
123	Trichloroethane, 1,1,2-	SecClar	A	RUN7	CT	CT	CT	CT	6.7E-01	1.0E+00	7.4E-02	1.1E-01
124	Trichloroethane, 1,1,2-	SecClar	D	RUN7	CT	HE	HE	CT	1.9E+01	3.0E+01	1.2E+01	1.9E+01
125	Trichloroethane, 1,1,2-	SecClar	B	RUN8	HE	HE	CT	CT	6.1E+00	9.4E+00	3.4E+00	5.3E+00
126	Trichloroethane, 1,1,2-	SecClar	C	RUN8	HE	CT	HE	CT	1.7E+00	2.6E+00	2.2E-01	3.5E-01
127	Trichloroethane, 1,1,2-	SecClar	B	RUN9	HE	HE	CT	CT	1.4E+01	2.1E+01	7.6E+00	1.2E+01
128	Trichloroethane, 1,1,2-	SecClar	C	RUN9	HE	CT	HE	CT	3.8E+00	5.8E+00	5.0E-01	7.8E-01

NA = not applicable. Values are NA for scenarios that were not evaluated (e.g., leachate from tanks or primary clarifiers).

Table C-4. Ratio of Leachate Concentration to Adjusted IWEM Protective Concentration for Risk = 1E-5

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Risk = 1E-5			
									Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose	Ingestion	Inhalation	Ingestion	Inhalation
1	Benzene	SI	A	RUN2	CT	CT	CT	CT	1.7E-02	1.9E-02	2.2E-03	2.5E-03
2	Benzene	SI	D	RUN2	CT	HE	HE	CT	4.4E-01	4.9E-01	3.2E-01	3.6E-01
3	Benzene	SI	F	RUN2	CT	HE	CT	HE	2.3E-01	2.6E-01	1.5E-01	1.7E-01
4	Benzene	SI	G	RUN2	CT	CT	HE	HE	7.3E-02	8.3E-02	1.2E-02	1.3E-02
5	Benzene	SI	B	RUN1	HE	HE	CT	CT	3.8E-01	4.3E-01	2.4E-01	2.8E-01
6	Benzene	SI	C	RUN1	HE	CT	HE	CT	1.2E-01	1.4E-01	1.9E-02	2.2E-02
7	Benzene	SI	E	RUN1	HE	CT	CT	HE	6.7E-02	7.6E-02	9.0E-03	1.0E-02
8	Benzene	SI	B	RUN3	HE	HE	CT	CT	1.8E+00	2.0E+00	1.1E+00	1.3E+00
9	Benzene	SI	C	RUN3	HE	CT	HE	CT	5.5E-01	6.3E-01	8.8E-02	1.0E-01
10	Benzene	SI	E	RUN3	HE	CT	CT	HE	3.1E-01	3.5E-01	4.2E-02	4.7E-02
11	Benzene	SI	B	RUN4	HE	HE	CT	CT	4.1E+00	4.7E+00	2.6E+00	3.0E+00
12	Benzene	SI	C	RUN4	HE	CT	HE	CT	1.3E+00	1.5E+00	2.1E-01	2.3E-01
13	Benzene	SI	E	RUN4	HE	CT	CT	HE	7.2E-01	8.1E-01	9.7E-02	1.1E-01
14	Benzene	SI	B	RUN5	HE	HE	CT	CT	2.3E-01	2.7E-01	1.5E-01	1.7E-01
15	Benzene	SI	C	RUN5	HE	CT	HE	CT	7.3E-02	8.3E-02	1.2E-02	1.3E-02
16	Benzene	SI	E	RUN5	HE	CT	CT	HE	4.1E-02	4.6E-02	5.5E-03	6.2E-03
20	Benzene	Tank	B	RUN1	HE	HE	CT	CT	NA	NA	2.9E+00	3.2E+00
21	Benzene	Tank	C	RUN1	HE	CT	HE	CT	NA	NA	2.2E-01	2.5E-01
22	Benzene	Tank	E	RUN1	HE	CT	CT	HE	NA	NA	1.1E-01	1.2E-01
23	Benzene	Tank	B	RUN3	HE	HE	CT	CT	NA	NA	4.7E+00	5.4E+00

(continued)

Table C-4. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Risk = 1E-5			
									Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose	Ingestion	Inhalation	Ingestion	Inhalation
24	Benzene	Tank	C	RUN3	HE	CT	HE	CT	NA	NA	3.7E-01	4.2E-01
25	Benzene	Tank	E	RUN3	HE	CT	CT	HE	NA	NA	1.7E-01	2.0E-01
26	Benzene	Tank	B	RUN5	HE	HE	CT	CT	NA	NA	1.8E-01	2.1E-01
27	Benzene	Tank	C	RUN5	HE	CT	HE	CT	NA	NA	1.4E-02	1.6E-02
28	Benzene	Tank	E	RUN5	HE	CT	CT	HE	NA	NA	6.7E-03	7.6E-03
29	Benzene	PrimClar	A	RUN7	CT	CT	CT	CT	NA	NA	1.1E-01	1.2E-01
30	Benzene	PrimClar	D	RUN7	CT	HE	HE	CT	NA	NA	1.6E+01	1.8E+01
31	Benzene	PrimClar	F	RUN7	CT	HE	CT	HE	NA	NA	7.3E+00	8.2E+00
32	Benzene	PrimClar	G	RUN7	CT	CT	HE	HE	NA	NA	5.7E-01	6.4E-01
33	Benzene	PrimClar	B	RUN8	HE	HE	CT	CT	NA	NA	4.7E+00	5.3E+00
34	Benzene	PrimClar	C	RUN8	HE	CT	HE	CT	NA	NA	3.7E-01	4.1E-01
35	Benzene	PrimClar	E	RUN8	HE	CT	CT	HE	NA	NA	1.7E-01	1.9E-01
36	Benzene	PrimClar	B	RUN9	HE	HE	CT	CT	NA	NA	4.7E+00	5.3E+00
37	Benzene	PrimClar	C	RUN9	HE	CT	HE	CT	NA	NA	3.7E-01	4.1E-01
38	Benzene	PrimClar	E	RUN9	HE	CT	CT	HE	NA	NA	1.7E-01	1.9E-01
55	Benzene	SecClar	A	RUN7	CT	CT	CT	CT	2.3E-02	2.6E-02	3.0E-03	3.4E-03
56	Benzene	SecClar	D	RUN7	CT	HE	HE	CT	5.9E-01	6.7E-01	4.3E-01	4.9E-01
57	Benzene	SecClar	F	RUN7	CT	HE	CT	HE	3.2E-01	3.6E-01	2.0E-01	2.3E-01
58	Benzene	SecClar	G	RUN7	CT	CT	HE	HE	1.0E-01	1.1E-01	1.6E-02	1.8E-02
59	Benzene	SecClar	B	RUN8	HE	HE	CT	CT	1.9E-01	2.2E-01	1.2E-01	1.4E-01
60	Benzene	SecClar	C	RUN8	HE	CT	HE	CT	6.1E-02	6.9E-02	9.7E-03	1.1E-02
61	Benzene	SecClar	E	RUN8	HE	CT	CT	HE	3.4E-02	3.8E-02	4.6E-03	5.1E-03

(continued)

Table C-4. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Risk = 1E-5			
									Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose	Ingestion	Inhalation	Ingestion	Inhalation
62	Benzene	SecClar	B	RUN9	HE	HE	CT	CT	4.3E-01	4.9E-01	2.7E-01	3.1E-01
63	Benzene	SecClar	C	RUN9	HE	CT	HE	CT	1.3E-01	1.5E-01	2.1E-02	2.4E-02
64	Benzene	SecClar	E	RUN9	HE	CT	CT	HE	7.6E-02	8.5E-02	1.0E-02	1.1E-02
89	Trichloroethane, 1,1,2-	SI	A	RUN2	CT	CT	CT	CT	3.0E-02	4.7E-02	3.3E-03	5.2E-03
90	Trichloroethane, 1,1,2-	SI	D	RUN2	CT	HE	HE	CT	8.8E-01	1.4E+00	5.6E-01	8.7E-01
91	Trichloroethane, 1,1,2-	SI	B	RUN1	HE	HE	CT	CT	6.5E-01	1.0E+00	3.6E-01	5.6E-01
92	Trichloroethane, 1,1,2-	SI	C	RUN1	HE	CT	HE	CT	1.8E-01	2.8E-01	2.4E-02	3.7E-02
93	Trichloroethane, 1,1,2-	SI	B	RUN3	HE	HE	CT	CT	3.0E+00	4.6E+00	1.7E+00	2.6E+00
94	Trichloroethane, 1,1,2-	SI	C	RUN3	HE	CT	HE	CT	8.3E-01	1.3E+00	1.1E-01	1.7E-01
95	Trichloroethane, 1,1,2-	SI	B	RUN4	HE	HE	CT	CT	7.8E+00	1.2E+01	4.4E+00	6.8E+00
96	Trichloroethane, 1,1,2-	SI	C	RUN4	HE	CT	HE	CT	2.2E+00	3.3E+00	2.9E-01	4.4E-01
97	Trichloroethane, 1,1,2-	SI	B	RUN5	HE	HE	CT	CT	4.0E-01	6.1E-01	2.2E-01	3.4E-01
98	Trichloroethane, 1,1,2-	SI	C	RUN5	HE	CT	HE	CT	1.1E-01	1.7E-01	1.5E-02	2.2E-02
101	Trichloroethane, 1,1,2-	Tank	B	RUN1	HE	HE	CT	CT	NA	NA	4.2E+00	6.5E+00
102	Trichloroethane, 1,1,2-	Tank	C	RUN1	HE	CT	HE	CT	NA	NA	2.8E-01	4.3E-01
103	Trichloroethane, 1,1,2-	Tank	B	RUN3	HE	HE	CT	CT	NA	NA	6.9E+00	1.1E+01
104	Trichloroethane, 1,1,2-	Tank	C	RUN3	HE	CT	HE	CT	NA	NA	4.6E-01	7.0E-01
105	Trichloroethane, 1,1,2-	Tank	B	RUN5	HE	HE	CT	CT	NA	NA	2.8E-01	4.3E-01
106	Trichloroethane, 1,1,2-	Tank	C	RUN5	HE	CT	HE	CT	NA	NA	1.8E-02	2.8E-02
107	Trichloroethane, 1,1,2-	PrimClar	A	RUN7	CT	CT	CT	CT	NA	NA	1.3E-01	2.1E-01
108	Trichloroethane, 1,1,2-	PrimClar	D	RUN7	CT	HE	HE	CT	NA	NA	2.3E+01	3.5E+01
109	Trichloroethane, 1,1,2-	PrimClar	B	RUN8	HE	HE	CT	CT	NA	NA	6.9E+00	1.1E+01

(continued)

Table C-4. (continued)

RunID	Chemical	WMU	Scenario	Water9 Run	High End Parameters				Risk = 1E-5			
									Leachate from WW Unit		Sludge in Landfill	
					Source	Fate	Exp	Dose	Ingestion	Inhalation	Ingestion	Inhalation
110	Trichloroethane, 1,1,2-	PrimClar	C	RUN8	HE	CT	HE	CT	NA	NA	4.5E-01	7.0E-01
111	Trichloroethane, 1,1,2-	PrimClar	B	RUN9	HE	HE	CT	CT	NA	NA	6.8E+00	1.1E+01
112	Trichloroethane, 1,1,2-	PrimClar	C	RUN9	HE	CT	HE	CT	NA	NA	4.5E-01	6.9E-01
123	Trichloroethane, 1,1,2-	SecClar	A	RUN7	CT	CT	CT	CT	6.7E-02	1.0E-01	7.4E-03	1.1E-02
124	Trichloroethane, 1,1,2-	SecClar	D	RUN7	CT	HE	HE	CT	1.9E+00	3.0E+00	1.2E+00	1.9E+00
125	Trichloroethane, 1,1,2-	SecClar	B	RUN8	HE	HE	CT	CT	6.1E-01	9.4E-01	3.4E-01	5.3E-01
126	Trichloroethane, 1,1,2-	SecClar	C	RUN8	HE	CT	HE	CT	1.7E-01	2.6E-01	2.2E-02	3.5E-02
127	Trichloroethane, 1,1,2-	SecClar	B	RUN9	HE	HE	CT	CT	1.4E+00	2.1E+00	7.6E-01	1.2E+00
128	Trichloroethane, 1,1,2-	SecClar	C	RUN9	HE	CT	HE	CT	3.8E-01	5.8E-01	5.0E-02	7.8E-02

NA = not applicable. Values are NA for scenarios that were not evaluated (e.g., leachate from tanks or primary clarifiers).
For 2-ethoxyethanol, only values for HQ =1 were calculated, and these are shown in Table C-3.